Characteristics of auto-ignition in a stratified iso-octane mixture with exhaust gases under homogeneous charge compression ignition conditions

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Ignition and propagation of a reaction front in a counterflow system of an iso-octane/air stream mixing with an exhaust gas stream is computationally investigated to understand the fundamental characteristics of homogeneous charge compression ignition (HCCI) auto-ignition. Various mixing rates are imposed on the system and the effects of dissipation rates on auto-ignition are studied. Ignition delay and front propagation speed across the mixing layer are determined as a function of a local mixture fraction variable. The results show that mixture inhomogeneity and dissipation rate have a significant influence on ignition. Diffusive transport is found to either hamper or advance ignition depending on the initial reactivity of the mixture. Based on the relative importance of diffusion on ignition front propagation, two distinct ignition regimes are identified: the spontaneous ignition regime and the diffusion-controlled regime. The transition between these two regimes is identified using a criterion based on the ratio of the timescales of auto-ignition and diffusion. The results show that ignition in the spontaneous regime is more likely under typical HCCI operating conditions with iso-octane due to its high reactivity. The present analysis provides a means to develop an improved modelling strategy for large-scale engine simulations.

1. Introduction

Homogeneous charge compression ignition (HCCI) engines have recently emerged as a viable choice for a next-generation internal combustion engine. In an HCCI engine, fuel and air are well mixed and induced into the engine cylinder. This charge is then compressed to a high pressure and temperature, which ignites the mixture without the need for an external ignition system. HCCI engines show a potential to combine the advantages of both spark ignition (SI) and compression ignition (CI) engines, in that the auto-ignition of reactants allows higher efficiencies, while the lean homogeneous mixture can substantially reduce the NOx and soot formation.

To understand the basic characteristics and to develop predictive design tools, there have been efforts to model the HCCI engine combustion with various levels of detail. So far, most of the modelling approaches employed either a simple zero-dimensional formulation [1–3], or a multi-zone model [4–6]. The zero-dimensional (0-D) model assumes that the entire combustion chamber is a well-stirred reactor with uniform temperature and composition,

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while the multi-zone model subdivides the engine into a number of zones in order to represent the in-cylinder temperature inhomogeneities. While computationally efficient and amenable to extensive parametric studies, these models neglect the effects of turbulence and mixing under the assumption that HCCI combustion is solely driven by chemical kinetics [7]. More recently, there have been limited attempts at tailoring the in-cylinder flow to achieve the desired operating conditions [8, 9]. These simplistic models, however, may lose accuracy in predicting the ignition and combustion processes when the effects of flow and mixing become significant.

One of the main challenges in the development of HCCI engines is to control the auto-ignition process and to achieve smooth energy release during the cycle. Unlike conventional engines, there is no direct control on the ignition timing in HCCI engines, such that the control has to be made by adjusting the intake charge conditions. Exhaust gas recirculation (EGR) has been considered an effective means to provide such a control strategy. With EGR, fresh reactants are mixed with exhaust gases which are at a slightly higher temperature but are deficient in reactants. Due to the high sensitivity of the reaction rates to temperature, even minor variations in the temperature distribution can help prevent an abrupt homogeneous explosion and allow smoother combustion. Recent simulation results [5] showed a strong correlation between temperature and mixture composition during the intake and compression stages, demonstrating that the temperature inhomogeneity within HCCI engines is primarily due to insufficient mixing with residual exhaust gases. Therefore, it is important to understand the effects of mixing and transport processes among the reactants and exhaust gases on the compression ignition behaviour.

The presence of mixture inhomogeneity leads to ignition and combustion characteristics that are fundamentally different from those expected in a perfectly homogeneous reactor. The local peaks in temperature and mixture composition can create ‘hot spots’ or kernels, which are more reactive than the rest of the mixture. Chemical reactions are thus initiated at the hot spots and subsequently propagate toward the neighbouring mixture in the form of a reaction front. Recent optical experiments with HCCI engines have demonstrated the existence of reaction fronts propagating at very high speeds [10, 11], thereby revealing the presence of different combustion regimes in HCCI engines. As a theoretical basis for the observed phenomena, Zeldovich [12] has identified three distinct regimes of a reaction front propagating through a non-uniform mixture: spontaneous propagation, normal detonation, and deflagration. The detonation regime is to be avoided for smooth engine operation, while the other two are of interest in the present context. Spontaneous propagation can be defined as consecutive events of spontaneous ignition at adjacent points, with different initial reactivities, which are perceived as a propagating reaction front. It is fundamentally different from a deflagration front in that transport processes between neighbouring points, such as heat and radical diffusion, are not necessary. Therefore, the propagation speed is not limited by the rate of diffusion and can be very high in magnitude compared to typical deflagration speeds. Bradley et al. [13], Gu et al. [14], and Chen et al. [15] have numerically examined these regimes of propagation and observed the presence of a spontaneous propagation mode with velocities much larger than the conventional diffusion-controlled flame. However, the role of these two regimes in the HCCI application is yet to be fully understood.

The main objective of the present study is to understand the effects of mixing on the overall ignition and subsequent front propagation characteristics. In particular, the ignition of a reactant stream mixed with exhaust gases under various mixing rates is systematically studied using a counterflow model considering iso-octane/air mixtures. Following the present authors’ earlier study using the methane–air system [16], the effects of the mixture fraction and scalar dissipation rates on ignition delay and front propagation speeds are investigated extensively, and different ignition regimes are identified. The results will provide a valuable
guidance to the development of improved multi-zone models or full-cycle simulations that can properly account for mixing and transport in HCCI combustion.

2. Problem configuration and numerical method

To investigate the parametric effects of the mixing between the fresh reactants and exhaust gases, a counterflow configuration is adopted where fresh reactants and the burned exhaust gases are supplied from each nozzle, forming a mixing layer near the stagnation plane. The nozzle velocities, which are kept identical on both sides, serve as an important parameter to adjust the rate of mixing, represented by the scalar dissipation rate ($\chi$). This study can be readily extended to different types of mixing, such as mixing between two reactant mixtures with different compositions, by imposing appropriate boundary conditions.

The governing equations for the counterflow configuration and details of the numerical implementation can be found in reference [17]. The steady solutions are obtained using a modified version of the Fortran program OPPDIF [18] and the unsteady solutions using OPUS [19]. These codes are interfaced with Chemkin [20] and Transport [21] for computing the reaction rates and transport properties. Iso-octane, which has ignition characteristics similar to gasoline, is chosen as the fuel for this study. The skeletal chemical kinetic mechanism for iso-octane ignition developed by Tanaka et al. [22] was used to compute the reaction rates. This mechanism was validated against experimental ignition delay times measured using a rapid compression machine [23]. It also agreed closely with the Lawrence Livermore National Laboratory (LLNL) detailed reaction mechanism for iso-octane combustion [24].

Premixed fuel/air mixture at an equivalence ratio of 0.3 flows through one nozzle against another stream of the corresponding products of combustion. Temperature at the fuel side inlet is held at 900 K and the hot exhaust inlet temperature at 1200 K. The nozzle velocities are set equal for all the cases discussed in this study. The nominal pressure of the system is set at 25 atm and is held constant during ignition. By considering a constant pressure system, the effects of compression heating have been neglected for the sake of simplicity. In a constant volume system, the heat released by early combustion will raise the pressure and heat up the end gas due to compression. This will increase the reactivity of the end mixture and shorten its ignition delay. While this is an important aspect of HCCI combustion, there is no suitable way of simulating constant volume combustion in the counterflow configuration, which is inherently an open system. A pressure rise in the system can be imposed by a prescribed pressure history independent of the actual ignition event. Rather than introducing an additional parameter into the problem, a constant pressure system has been chosen for this study. The results are expected to address adequately the fundamental characteristics of the development of ignition fronts in an early stage.

3. Results and discussion

3.1 Mixture fraction variable

In this study, the adiabatic mixing of fresh reactants with their burned products is considered, such that a mixture fraction variable, $Z$, can be defined to characterize the level of mixing. The mixture fraction is a conserved scalar which, under assumption of unity Lewis numbers, can be used uniquely to represent the local mixture composition and enthalpy. If the fresh reactants and burned products are mixed without chemical reaction in the ratio $Z : (1 - Z)$,
the resultant mixture composition is

\[ Y_k = Z Y_{k,R} + (1 - Z) Y_{k,E}. \]  

(1)

where \( Y_k \) is mass fraction of species \( k \) and subscripts \( R \) and \( E \) denote the reactant and exhaust streams, respectively. Similarly, temperature of the mixture can be determined by adiabatically mixing the enthalpies of the two streams as

\[ h = Z h_R + (1 - Z) h_E. \]  

(2)

Therefore, any given value of \( Z \) uniquely determines the composition and the enthalpy of the mixture.

### 3.2 Homogeneous ignition delay

The main interest of this study is to assess the effects of mixing and transport on the ignition at various locations within the mixing layer. For the purpose of analysis, a reference case is considered where ignition at any local point within the mixing layer is described by homogeneous explosion of a uniform mixture at an identical condition. This corresponds to Zeldovich’s spontaneous propagation regime, which can be readily simulated by a series of SENKIN [25] calculations using detailed iso-octane chemistry. Assuming unity Lewis numbers for all species, the initial composition and enthalpy at any location in the mixing layer is uniquely determined as a function of the mixture fraction by equations (1) and (2). Using these initial conditions, the ignition delay is computed for different values of \( Z \) using a homogeneous model and is shown in figure 1 as a dashed curve. Here the ignition delay is defined as the time at which 20 percent of the total heat release is generated.

Since the Lewis number of iso-octane is greater than unity, an alternative and more accurate reference case is obtained by considering the actual initial composition and enthalpy conditions taken from a steady frozen counterflow calculation employing detailed transport properties. The results are plotted in figure 1 as a solid curve, showing a quantitative difference compared

![Figure 1. Computed homogeneous auto-ignition delays as a function of Z. Also shown is the molar composition of the mixtures at Z = 0 and 1.](image-url)
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to those based on the equal-diffusivity assumption. The solid curve prediction is defined as a reference 0-D ignition delay, \( \tau_{i,0}(Z) \), and will be used in comparison with the counterflow ignition results in the presence of mixing and dissipation.

Figure 1 shows that the ignition is very slow at \( Z = 0 \) due to the absence of reactants, and at \( Z = 1 \) due to the low temperature. Consequently, there exists a value, \( Z_{\text{min}} \), at which the minimum ignition delay is obtained. Due to the higher sensitivity of reaction to temperature, the minimum ignition delay is obtained at a location closer to the exhaust gas side at \( Z_{\text{min}} \approx 0.15 \).

3.3 Steady ignition limit

The ignition of the counterflow mixing layer under various scalar dissipation rates is now studied. Before proceeding with the unsteady ignition calculation, it is necessary to identify the maximum nozzle velocity below which ignition can occur. The steady ignition limit, known as the ignition turning point, is determined by successively computing steady frozen solutions as the nozzle velocities are reduced. Figure 2 shows the response of maximum temperature in the mixing layer as a function of the nozzle velocity. A turning point occurs at \( V = 146 \text{ cm/s} \), which is the steady ignition limit. For velocities above this limit, the reactions are suppressed due to insufficient residence time and thus a frozen steady solution is obtained. Therefore, the mixture is ignitable only for velocities below this limit.

It is noteworthy that the frozen branch in figure 2 shows that the maximum temperature rises as much as 100 K before the ignition turning point is reached. This was found to be a unique characteristic of the low-temperature chemistry associated with higher hydrocarbon fuels, known as the cool flame phenomenon. Figure 3 shows the temperature and H-atom concentration profiles for the two solutions at \( V = 147 \text{ cm/s} \), as marked in figure 2. The duality of the solutions at the same nozzle velocity represents a weakly burning cool flame in the lower branch (L) and an intensely burning flame in the upper branch (U). Although the overall shapes of the profiles look similar, a large difference in the peak radical concentration

Figure 2. Steady ignition turning point behaviour.
is clearly observed. Since the ignition to the intensely burning state is of practical interest, the cool flame behaviour is not considered further in the analysis of the ignition characteristics.

3.4 Effects of mixing rate on ignition

To study the effects of scalar dissipation rate induced by the flow strain, unsteady calculations of the ignition events are undertaken as follows. First, a frozen solution for a chosen velocity in an ignitable condition ($V < 146 \text{ cm/s}$) is obtained by artificially suppressing all the reaction rates. This solution is then imposed as the initial condition and the unsteady simulation started with chemical reactions turned on. Figures 4 and 5 show the evolution of temperature profile...
Figure 5. Temporal evolution of the temperature profile during the ignition event, for $V = 5$ cm/s (in the mixture fraction coordinate).

plotted in the physical coordinate, $x$, and the mixture fraction space, $Z$, respectively, at a nozzle inlet velocity of 5 cm/s. It is seen that the temperature rise initially originates from a location close to the hot exhaust stream, consistent with the homogeneous ignition results in figure 1. As the ignition kernel further develops, however, the temperature peak shifts to the fresh reactant stream, exhibiting a reaction front propagation. It is evident that the ignition behaviour of any local point is not purely independent but is influenced by the neighbouring mixture conditions through the diffusion of heat and radicals.

Using the full transient solutions, the history of a mixture at a specific value of $Z$ is monitored and the ignition delay is determined as a function of $Z$. The ignition delay in the presence of heat and radical transport, $\tau_i$, is defined as the time at which 20 percent of the total heat release has occurred. Therefore, a single run of unsteady calculation yields a mapping of $\tau_i(Z)$ that can be compared with the reference case shown in figure 1. The process is repeated at increasing nozzle velocities, which steepens the gradients in the mixing layer and increases the scalar dissipation rate. Figure 6 shows the ignition delay ($\tau_i$) as a function of $Z$ for various nozzle velocities. The reference 0-D result $\tau_{i,0}(Z)$ is also plotted for comparison. The results show that the ignition delay in the presence of transport is longer compared to the homogeneous prediction for approximately $0.1 < Z < 0.7$, and is shorter elsewhere. This clearly demonstrates that the mixing rate can either favourably or adversely affect the ignition depending on the local mixture condition.

The observed behaviour has the following physical implication. When the mixture is unreactive either due to the lack of reactants (small $Z$) or due to the low temperature (large $Z$), the exchange of reactants and radicals from the neighbouring mixture promotes ignition. On the other hand, if the initial mixture is reactive (intermediate values of $Z$), mixing and transport result in a loss of enthalpy and radicals from the ignition kernel, hence retarding ignition compared to the homogeneous counterpart. As expected, these effects are more pronounced when the nozzle velocity and consequently the scalar dissipation rate is increased. Note that the crossover of the curves near $Z = 0.1$, which was not observed in the current authors’ earlier study with a methane–air system [16], is due to the low diffusivity of iso-octane so that the fuel does not further penetrate into the hotter boundary. However, the ignition behaviour near the exhaust gas stream is of little practical significance since the total temperature rise itself
is very small at this location. Therefore, it is concluded that the overall effect of mixing is to ‘even out’ the disparities in the ignition delays arising from the initial mixture stratification by allowing the more reactive mixture pockets to ‘help out’ the neighbouring less reactive mixture pockets.

3.5 Front propagation speed

As shown in figures 4 and 5, the ignition event in a mixing layer is manifested as a propagation of reaction front from the exhaust gas stream towards the colder reactant mixture. Therefore, it is of interest to examine the propagation speed as a characteristic of the overall heat release rate and reactivity of the mixture. Knowing the spatial ignition delay distribution, \( \tau_i(x) \), from the results of the unsteady counterflow calculation, a propagation speed for the ignition front can be defined as

\[
S_f = \left( \frac{d\tau_i}{dx} \right)^{-1} = \left( \frac{d\tau_i}{dZ} \cdot \frac{dZ}{dx} \right)^{-1}.
\]

(3)

Therefore, \( S_f \) can be determined either directly by evaluating \( d\tau_i/dx \) in the physical space or by using the chain rule, \( d\tau_i/dx = (d\tau_i/dZ) \times (dZ/dx) \), in the mixture fraction space with the knowledge of \( Z(x) \).

To assess the effects of transport on \( S_f \), a reference propagation speed based on the 0-D calculation can be determined by

\[
S_{f,0} = \left( \frac{d\tau_{i,0}}{dZ} \cdot \frac{dZ}{dx} \right)^{-1},
\]

(4)

where \( S_{f,0} \) represents the front propagation speed in Zeldovich’s spontaneous propagation regime, that is the hypothetical front speed for the same \( Z(x) \) distribution in the mixing layer in the absence of mixing and dissipation. The difference between \( S_f \) and \( S_{f,0} \) indicates the
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Figure 7. Reaction front speed $S_f$ (symbols) and $S_{f0}$ (line) as a function of $Z$.

additional effect of mixing and transport on ignition front propagation. In the Appendix, an explicit expression for $d\tau_{i0}/dZ$ using one-step chemistry is derived by an asymptotic analysis for further discussion.

Figure 7 shows a comparison between the $S_f$ (symbols) and $S_{f0}$ (line) at nozzle velocities of 5 and 130 cm/s. For very low values of $Z$ ($<0.1$), the temperature rise during ignition is so small that numerical evaluation of $S_f$ has no practical significance. At a low scalar dissipation rate ($V = 5$ cm/s), the two propagation speeds are in good agreement, implying that the ignition behaviour is little affected by mixing and thus can be described as a series of homogeneous ignition events.

At higher mixing rate ($V = 130$ cm/s), however, the difference between $S_f$ and $S_{f0}$ becomes significant. In particular, it is of interest to note that $S_f$ can be slower or faster than $S_{f0}$ depending on the range of $Z$ ($Z \approx 0.7$ is the crossover point for this case). As observed in figure 6, mixing tends to even out the reactivity across the mixing layer by transporting the enthalpy and radicals from more reactive (higher $T$ and lower $Z$) to less reactive (lower $T$ and higher $Z$) mixture. More importantly, unlike $S_{f0}$ which decreases monotonically over a wide range of $Z$ (say $0.2 < Z < 0.9$), $S_f$ levels off at approximately 3 cm/s. As shown in the Appendix, in the homogeneous ignition limit the ignition delay is uniquely determined by the local mixture fraction, such that the propagation speed, which is proportional to $(d\tau_{i0}/dZ)^{-1}$, decays exponentially with $Z$. Therefore, the $S_f$ behaviour for the high mixing rate condition shows a clear deviation from the pure spontaneous front propagation. As suggested by Zeldovich [12], if the mixture reactivity is such that a spontaneous ignition front can only propagate at very low speeds, then a deflagration front driven by the molecular diffusion process becomes the overriding propagation mechanism. This is referred to as the diffusion-controlled regime of ignition. The results in figure 7 thus demonstrate that a transition in the ignition characteristics can occur within the mixing layer in the presence of steep gradients and large dissipation rates. These results agree with the authors’ previous two-dimensional direct numerical simulation (DNS) study, in which a diffusion-controlled propagation mode was observed at regions of high temperature gradient [26].
It should be noted that the above observation does not necessarily imply that flame propagation occurs in real HCCI engines. The diffusion-controlled ignition behaviour may not occur in HCCI engines under practical operating conditions for the following reasons.

1. In the presence of radiative heat loss, which was not considered in this study, the typical mixture composition may fall under the lean flammability limit, and a flame-like front propagation may not be sustainable.
2. Compression of the end gas due to heat release will increase its reactivity and promote spontaneous ignition, thereby reducing the chances and duration of a diffusion-controlled front propagation.

A more rigorous criterion to distinguish the different ignition regimes is proposed in the next section.

### 3.6 Ignition regimes

Identifying two different ignition regimes, the spontaneous ignition regime and the diffusion-controlled regime, is important in HCCI modelling since the two ignition regimes have a fundamentally different response to the imposed system parameters. Therefore, different modelling strategies are needed to develop the ignition submodels for the device-level simulations of the HCCI combustion. In this section, a criterion is proposed to distinguish the two ignition regimes.

Determining the criterion for the two regimes comes from the observation that one is dominated by spontaneous chemical reaction while the other by diffusional preheating. Therefore, the most obvious consideration is the characteristic timescales of diffusion and spontaneous propagation processes. First, define a characteristic length scale, $\Delta x$, based on the flow strain rate, $\kappa$, and thermal diffusivity, $\alpha$, as

$$\Delta x = \sqrt{\alpha/\kappa},$$  

which can be converted to the mixture fraction space using the relations $\Delta Z = \Delta x \cdot (dZ/dx)$ and $\chi = \alpha(dZ/dx)^2$ to obtain

$$\Delta Z = \sqrt{\chi/\kappa}. \quad (6)$$

The timescale of diffusion across $\Delta Z$ is then given by

$$\tau_d = \frac{\Delta Z^2}{\chi}. \quad (7)$$

As for the spontaneous propagation regime, the time taken by the ignition wave to traverse the same distance is

$$\tau_{sp} = \frac{d\tau_{i,0}}{dZ} \Delta Z. \quad (8)$$

The ratio of these two timescales is defined as the transition parameter:

$$\beta = \frac{\tau_{sp}}{\tau_d} = \frac{\chi \cdot d\tau_{i,0}}{\Delta Z \cdot dZ}. \quad (9)$$

Note that the transition parameter has a similar form as the reduced Damköhler number, equation (A21), derived in the asymptotic analysis in the Appendix, thereby further confirming the relevance in representing the characteristic system Damköhler number. For $\beta < 1$, the time needed for spontaneous propagation is much shorter than the diffusion timescale, such that ignition is in the spontaneous propagation regime. On the other hand, for $\beta > 1$, the timescale
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3.7 Parameterization of mixing effects

In the previous section, it was found that the ignition characteristics of a mixing layer between fuel–air and exhaust gases depend primarily on two physical parameters, namely the mixture fraction ($Z$), which represents the degree of mixing, and the scalar dissipation rate ($\chi$), which is a measure of the rate of mixing. This has a significant implication in the current approaches to full-cycle engine simulations. While a multi-zone model for HCCI modelling takes into account the degree of mixing, the mixing rate information is often neglected. Recognizing the importance of the two mixing parameters, $Z$ and $\chi$, an improved predictive submodel for HCCI ignition is proposed. For a given set of enthalpy and composition conditions for the reactant and exhaust gases, the counterflow calculation results can be used to map out the ignition delay as a function of the two parameters.

Figure 9 shows an example of such a mapping based on the extensive calculations shown in figure 6. The contour plot clearly indicates the general trend that the ignition delay becomes longer as the mixture fraction and the scalar dissipation rate increase. The dashed line indicates the computed transition boundary between the spontaneous propagation and the diffusion-controlled regimes, as defined in the previous section. It is seen that the region of diffusion is shorter and the ignition front propagates as a diffusion-controlled wave, whose speed is enhanced by the effect of mixing and transport. Figure 8 shows the computed values of $\beta$ for various nozzle velocity conditions. The $\beta = 1$ line denotes the crossover point between the two ignition regimes. The results clearly indicate that ignition is predominantly in the spontaneous propagation regime when the nozzle velocity is low. However, as the scalar dissipation rate increases, a larger fraction of the mixture (at higher $Z$) behaves as the diffusion-controlled propagation regime. In particular, for $V = 130 \text{ cm/s}$, a significant fraction of the mixture ($Z > 0.5$) falls into the diffusion-controlled regime, demonstrating the significance of the mixedness ($Z$) as well as the rate of mixing ($\chi$) in determining the ignition characteristics.
occupied by the spontaneous propagation mode becomes narrower as the scalar dissipation rate increases. A parameteric mapping as shown in figure 9 provides valuable insights about the characteristics of ignition in the HCCI system in the presence of strong concentration and enthalpy fluctuations. Furthermore, these types of pre-generated one-dimensional (1-D) data can be used as a tabulated submodel to predict ignition in HCCI engines using multi-zone or KIVA simulations. Implementation of the proposed concept in KIVA application is currently in progress.

4. Conclusions

Numerical simulations were performed in a counterflow configuration by allowing a stream of fresh iso-octane/air mixture flow against burned exhaust products. The ignition delay and front propagation speed across the mixing layer were determined as a function of a local mixture fraction variable as well as the scalar dissipation rate. It was found that the rate of mixing has a significant effect on the overall ignition characteristics, by favourably or adversely affecting the ignition behaviour depending on the initial reactivity of the mixture. Two different regimes of ignition front propagation were identified and a criterion to distinguish the two regimes was proposed based on the characteristic timescales of homogeneous ignition and the mixing rate. The present results provide insights in understanding fundamental ignition characteristics within HCCI engines. The concept of parameterization based on the mixture fraction and scalar dissipation rate suggest potential ignition submodels that can be used in full-cycle engine simulations.

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A ppendix

To understand the basic characteristics of ignition in the mixing layer, an asymptotic analysis is performed to obtain simple closed-form solutions. The energy equation governing the counterflow system can be rewritten in terms of the mixture fraction variable as

$$\frac{\partial T}{\partial t} = \chi \frac{\partial^2 T}{\partial Z^2} + \dot{\omega},$$  \hspace{1cm} (A1)

where $\chi = \alpha (\nabla Z)^2$ is the imposed scalar dissipation rate and $\alpha$ is the thermal diffusivity. A one-step irreversible chemical reaction with an activation energy $E$ is used to obtain the following expression for the chemical heat release term:

$$\dot{\omega} = \left( \frac{Q}{\rho C_p} \right) A Y_f \exp \left[ -\frac{E}{RT} \right],$$  \hspace{1cm} (A2)

where $Q$ is the heat of reaction, $\rho$ is the density of the mixture, $C_p$ is the specific heat, $A$ is the pre-exponential factor, $Y_f$ is the mass fraction of fuel, and $R$ is the universal gas constant.

For simplicity, the Lewis number is assumed to be unity and the coupling function is defined as

$$T + \frac{Q}{\rho C_p} Y_f = T_0 + \frac{Q}{\rho C_p} Y_{f,0},$$ \hspace{1cm} (A3)

where the initial conditions $T_0(Z)$ and $Y_{f,0}(Z)$ are specified using the mixture fraction relations in equations (1) and (2). Therefore, the chemical heat release term is rewritten as

$$\dot{\omega} = A \left( T_0 + \frac{Q}{\rho C_p} Y_{f,0} - T \right) \exp \left[ -\frac{E}{RT} \right].$$ \hspace{1cm} (A4)

Introducing non-dimensional variables

$$\theta = \frac{T}{T_E}, \hspace{1cm} \tau = \frac{t}{\tau_{i,0}}, \hspace{1cm} \tilde{\chi} = \chi \tau_{i,0}, \hspace{1cm} \tilde{A} = A \tau_{i,0},$$ \hspace{1cm} (A5)

where $\tau_{i,0}$ is the ignition delay to be determined later, and defining additional parameters

$$\mu = (T_E - T_R)/T_E, \hspace{1cm} \beta = Q Y_{f,R}/\rho C_p T_E - \mu, \hspace{1cm} \epsilon = R T_E / E,$$ \hspace{1cm} (A6)

equation (A1) is written as

$$\frac{\partial \theta}{\partial \tau} = \tilde{\chi} \frac{\partial^2 \theta}{\partial Z^2} + \tilde{A}(1 + \beta Z - \theta) \exp \left[ -\frac{1}{\epsilon \theta} \right].$$ \hspace{1cm} (A7)

The above equation is subject to the boundary condition

$$\theta(Z = 0, \tau) = 1; \hspace{1cm} \theta(Z = 1, \tau) = 1 - \mu,$$ \hspace{1cm} (A8)

and the initial condition

$$\theta(Z, \tau = 0) = \theta_0(Z) = 1 - \mu Z.$$ \hspace{1cm} (A9)
To obtain the reference homogeneous ignition model, the diffusion term is neglected by assuming that $\tilde{\chi}$ is small, yielding
\[
\frac{d\theta}{d\tau} = \tilde{A}(1 + \beta Z - \theta) \exp\left[-\frac{1}{\epsilon \theta}\right],
\]
(A10)
such that the thermal runaway time can be determined as a function of $Z$. The temperature is expanded about its initial condition in terms of the small parameter $\epsilon$ as \[8\],
\[
\theta(Z) = \theta_0(Z) + \epsilon \theta_1(t) + O(\epsilon^2) = (1 - \mu Z) + \epsilon \theta_1 + O(\epsilon^2).
\]
(A11)
Substituting the expansion (A11) into equation (A10) yields the equation at leading order in $\epsilon$:
\[
\frac{d\theta_1}{d\tau} = \tilde{A}(\beta + \mu)Z \exp\left[-\frac{1}{\epsilon (1 - \mu Z)}\right] \exp\left[\frac{\theta_1}{(1 - \mu Z)^2}\right],
\]
(A12)
with the initial condition, $\theta_1(\tau = 0) = 0$. Equation (A12) is readily integrated to yield the solution
\[
\theta_1 = (1 - \mu Z)^2 \log \left[\frac{1}{1 - \tau}\right],
\]
(A13)
if the ignition time, $\tau_{i,0}$, is defined as
\[
\tau_{i,0}(Z) = \frac{\epsilon (1 - \mu Z)^2}{A(\beta + \mu)Z} \exp\left[\frac{1}{\epsilon (1 - \mu Z)}\right].
\]
(A14)
The solution $\theta_1$ goes to infinity at $\tau = 1$, or $t = \tau_{i,0}$. This implies that mixtures of different $Z$ ignite at different instants given by $\tau_{i,0}(Z)$.

The point of shortest ignition delay can be obtained by setting $d\tau_{i,0}/dZ = 0$. Differentiating (A14), we obtain
\[
\frac{d\tau_{i,0}}{dZ} = \frac{1}{A(\beta + \mu)Z} \exp\left[\frac{1}{\epsilon (1 - \mu Z)}\right] \left\{\mu - \epsilon - \frac{1 - \mu^2 Z^2}{Z}\right\}.
\]
(A15)
In the limit of small $\epsilon$, $d\tau_{i,0}/dZ = 0$ happens for $Z_{\text{min}} = \epsilon/\mu$, which is the location in $Z$ of the shortest ignition delay. The small value of $Z_{\text{min}}$ reflects the exponential dependence of reactivity on temperature, and is consistent with the results shown in figure 1.

In the context of determining the front propagation speed using equation (4), the explicit expression as equation (A15) is useful. For the majority of the mixing layer of interest, $Z = O(1) \gg Z_{\text{min}}$, the approximation
\[
\frac{d\tau_{i,0}}{dZ} = \frac{\mu}{A(\beta + \mu)Z} \exp\left[\frac{1}{\epsilon (1 - \mu Z)}\right]
\]
(A16)
is valid. Using (A16), the energy equation (A17) can be rewritten in terms of the homogeneous ignition delay as
\[
\frac{\partial \theta}{\partial \tau} = \tilde{\chi} \frac{\partial^2 \theta}{\partial Z^2} + \mu \tau_{i,0} \left(\frac{d\tau_{i,0}}{dZ}\right)^{-1} \frac{(1 + \beta Z - \theta)}{(\beta + \mu)Z} \exp\left[\frac{\theta - (1 - \mu Z)}{\epsilon (1 - \mu Z) \theta}\right].
\]
(A17)
For asymptotic analysis, substituting the expansion (A11) in (A17), the leading order equation in $\epsilon$ becomes
\[
\frac{\partial \theta_1}{\partial \tau} = \tilde{\chi} \frac{\partial^2 \theta_1}{\partial Z^2} + \frac{\mu \tau_{i,0}}{\epsilon} \left(\frac{d\tau_{i,0}}{dZ}\right)^{-1} \exp\left[\frac{\theta_1}{(1 - \mu Z)^2}\right].
\]
(A18)
The two terms on the right-hand side of equation (A18), respectively, represent the energy loss and source of ignition. In other words, the solution to the steady equation
\[
\tilde{\chi} \frac{\partial^2 \theta}{\partial Z^2} + \frac{\mu \tau_{i,0}}{\epsilon} \left( \frac{d \tau_{i,0}}{dZ} \right)^{-1} \exp \left[ \frac{\theta_1}{(1 - \mu Z)^2} \right] = 0 \quad (A19)
\]
represents the steady frozen solution for the reactive–diffusive system, and can be written as
\[
\frac{\partial^2 \theta}{\partial Z^2} + D \exp \left[ \frac{\theta_1}{(1 - \mu Z)^2} \right] = 0 \quad (A20)
\]
where \( D \) is the reduced Damköhler number defined as:
\[
D = \frac{\mu}{\epsilon \tilde{\chi}} \left( \frac{d \tau_{i,0}}{dZ} \right)^{-1} = \frac{Z_{\min}^{-1}}{\chi} \left( \frac{d \tau_{i,0}}{dZ} \right)^{-1}. \quad (A21)
\]
The steady system (A19) shows an ignition turning point at \( D = O(1) \) condition. The reduced Damköhler number represents the ratio of the chemical source intensity to the dissipation loss, and is used as a key parameter to characterize the ignition regimes.

References


