The effects of non-uniform temperature distribution on the ignition of a lean homogeneous hydrogen–air mixture

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Abstract

To characterize the ignition process in homogeneous charge compression ignition engines, high fidelity simulations are performed to study the effects of different initial temperature distributions on the autoignition of a turbulent homogeneous mixture at high pressure. The effects of the initial temperature distribution on the ignition and subsequent heat release are studied by comparison of simulations with three initial random temperature fields having different skewness. It is found that the scalar mixing and turbulence have a significant influence on the initial location and further evolution of the ignition kernels. A comparison of the integrated heat release rates shows that the presence of a hot core leads to early ignition and increased duration of burning, while a cold core leads to a dormant end gas, which is consumed by slow combustion. The extent of flame fronts is quantified by a temperature gradient cut-off, revealing distinct behavior in the appearance of flame fronts for the three cases. Finally, two distinct ignition regimes, namely the spontaneous propagation and the deflagration regimes, are identified, and a predictive criterion is defined based on the spontaneous propagation speed and deflagration speed at the local mixture conditions. The predictions are found to be consistent with the observed results, suggesting a potential strategy in the modeling of HCCI combustion process.

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1. Introduction

The concept of homogeneous charge compression ignition (HCCI) engines has attracted significant research interests in recent years as an alternative IC engine design with promises for high efficiency and low emissions. In HCCI engines, the reactant charges are very lean and nearly homogeneous, hence the ignition and combustion processes are believed to be primarily controlled by the kinetically driven processes. As such, one of the key challenges in the development of HCCI engines is to control the start of combustion and to ensure smooth heat generation during the cycle under a wide range of load conditions. To overcome the technical challenges and to assist the development of the HCCI engines,
accurate predictive simulations of the ignition and subsequent combustion processes in an HCCI-like environment are important. However, a full three-dimensional simulation that includes detailed chemical kinetic models and turbulence is beyond the capabilities of the computational resources in the foreseeable future [1]. Consequently, most of the previous modeling work incorporating detailed chemistry employed either zero-dimensional or multi-zone models [2] that divide the combustion chamber into a finite number of isolated zones. These models are based on the assumption that turbulence and mixing have little effect during the rapid ignition process in HCCI engines.

Despite the conceptual framework that HCCI combustion is anticipated to be nearly homogeneous, however, there are experimental observations suggesting that ignition and combustion processes in HCCI engines are far from homogeneous [3]. Non-uniform ignition events arising from local “hot spots” have also been reported [4]. Partial mixture stratification in an HCCI engine can also be achieved using exhaust gas recirculation, which is considered a feasible means to control the start of combustion and prolong the burning duration [5]. Therefore, it is of practical importance to understand and to characterize the autoignition process of a nearly homogeneous lean mixture subjected to fluctuations in flow and scalar fields, such that the overall impact of the turbulence and mixing on the ignition behavior is fully accounted for.

Another notable issue in recent experimental studies is the observation of a flame-like wave propagation in HCCI engines [3,6]. Although these experiments strongly support the presence of reaction front propagation, it is unclear whether the observed front indeed represents a deflagration wave. In an earlier work, Zeldovich [7] identified three distinct regimes of a reaction front propagating through a non-uniform mixture: spontaneous propagation, normal detonation, and deflagration. The ignition front propagation arising from the hot spots in HCCI engines can also be described using a similar approach, as in Gu et al. [8]. Such a classification of different ignition regimes under various engine operating conditions will provide valuable insights into the modeling of HCCI ignition and combustion.

Therefore, the objective of the present study was to perform high-fidelity simulations of the ignition of a homogeneous lean mixture in the presence of turbulence and non-uniform temperature distribution, as a canonical problem to unravel some fundamental issues related to ignition in an HCCI-like environment. Using two-dimensional calculations with detailed hydrogen–air chemistry under high-pressure conditions, the effects of different temperature distributions on the overall ignition behavior are investigated. A criterion to distinguish two ignition regimes, namely the spontaneous propagation and deflagration, is proposed and applied to the simulation data to identify the ignition characteristics in HCCI applications.

2. Numerical method and initial conditions

The autoignition of two-dimensional turbulent lean hydrogen–air mixture is computed using direct numerical simulation in a closed volume at high pressure conditions to represent the compression ignition process in an HCCI engine. The full compressible Navier–Stokes, species, and energy equations for a reacting gas mixture are solved using a fourth-order Runge–Kutta method for time integration and an eighth-order explicit spatial differencing scheme [9,10]. The chemical mechanism for hydrogen–air oxidation developed by Mueller et al. [11] with 9 species and 19 reversible reactions is used. The hydrogen chemistry is adopted for its simplicity in computation, yet the consideration of detailed intermediate species will allow us to study generic responses of a system that can serve as a building block for more complex hydrocarbon fuels. The mixture specific heat is determined locally as a function of mixture composition; that is, 

\[ C_p = \sum C_{p,k} Y_k \]

where each \( C_{p,k} \) is curve-fitted as a function of temperature using the Chemkin thermodynamic database [12]. The molecular viscosity is temperature-dependent, and constant Lewis numbers for individual species are determined for the mixture at 1000 K.

The computational domain is a two-dimensional square of size 4.1 mm on each side. A 960 × 960 grid is used, which gives us an effective spatial resolution of 4.3 μm. Such a fine resolution is necessary to fully resolve the intermediate species profiles for the high temperatures and pressures considered. Periodic boundary conditions are imposed on all four sides of the domain to reproduce the constant volume combustion process.

A turbulent flow field is superimposed as the initial condition by using a prescribed kinetic energy spectrum function [13]. The integral scale of turbulence computed from a two-point velocity correlation, \( L_{11} \), is 0.34 mm, and the turbulence intensity is \( u' = 0.5 \text{ m/s} \). The pressure is set at 41 atm, and a lean hydrogen–air mixture at an equivalence ratio of 0.1 is used uniformly throughout the domain. The mixture composition is chosen to be leaner than a typical HCCI engine condition to prevent excessive pressure rise and compression heating effects. An energetic hydrogen–air mixture at higher equivalence ratio may lead to the formation of a detonation wave, which cannot be resolved on the grid used in this work.

Since the main objective of the study was to investigate the effects of temperature inhomogene-
ity, the aforementioned initial conditions for flow, pressure, and mixture composition are common for all the cases studied, and three different initial temperature distributions are considered. Case A, which is the baseline case, has an initial temperature field \( T_0 \) given by \( T_0(x,y) = \bar{T}_0 + T_0(x,y) \), where \( \bar{T}_0 \) is the mean temperature and \( T_0(x,y) \) is a prescribed turbulent temperature field using a similar method as the turbulence energy spectrum. However, there is no correlation between the temperature and turbulence fields. The mean of \( T_0(x,y) \) is set to zero. Cases B and C are obtained by superimposing a bell-shaped function over Case A, thereby generating a hot/cold core gas at the center of the domain. The temperature field for Cases B and C is given by, \( T_0(x,y) = \bar{T}_0 + T_0(x,y) + \tilde{T}_0(x,y) \), where

\[
\tilde{T}_0(x,y) = \frac{A}{\pi} \exp\left( -\frac{2n^2r^2}{l^2} \right) - \frac{A}{2n^2}, \tag{1}
\]

In the above equation, \( l \) is the length of the domain, \( r^2 = (x-x_c)^2 + (y-y_c)^2 \), \((x_c,y_c)\) is the center of the hot or cold core gas, \( n \) is a scale factor that determines the size of the core, and \( A \) is the amplitude of the function. The sign of \( A \) determines whether the core gas is hotter or colder than that for the baseline case. Here, the initial conditions for Cases B and C are set with \( n = 4 \), \( A = 50 \) and \( -50 \), respectively, such that the amplitude of \( T_0 \) is approximately 16 K. By definition, \( \bar{T}_0 \) has a zero mean so that the mean of the total temperature distribution remains at \( \bar{T}_0 \).

For all cases, the mean temperature is held at 1070 K, and the amplitude of \( T_0 \) is modulated to obtain a standard deviation of 15 K. Table 1 lists the maximum and minimum temperatures along with \( R_T \), the ratio of the area of domain with \( T_0 > \bar{T}_0 \) to the area with \( T_0 < \bar{T}_0 \). Clearly, the values of \( R_T \) for Cases B and C indicate that the temperature distribution is skewed towards the hotter and colder sides, respectively, with the same mean temperature. The functional form of \( \tilde{T}_0 \) also ensures that the hotter/colder core gas is relatively insulated from the rest of the mixture, hence preventing the early dissipation of the peak/trough temperature out during the induction period. The pressure and mean temperature have been chosen to mimic the conditions at top dead center of an engine with a compression ratio of 14. Numerical solutions typically required time steps of the order of \( 1 \times 10^9 \) s and 80,000 h of CPU time for each case on IBM SP2 processors.

### Table 1

<table>
<thead>
<tr>
<th>Case</th>
<th>( T_{0,\text{max}} ) (K)</th>
<th>( T_{0,\text{min}} ) (K)</th>
<th>( R_T )</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>1106</td>
<td>1023</td>
<td>0.98</td>
</tr>
<tr>
<td>B</td>
<td>1111</td>
<td>1028</td>
<td>0.87</td>
</tr>
<tr>
<td>C</td>
<td>1100</td>
<td>1003</td>
<td>1.17</td>
</tr>
</tbody>
</table>

**Fig. 1. Reference case ignition delays.** For isolated cells, symbols show the 1D numerical result, and dashed line shows the correlation from Eq. (4).
\[ \tau_{ic} = 8.834 \times 10^{-13} \exp \left( \frac{23,000}{T_0} \right) \text{[s]}, \quad (2) \]

for the pressure-coupled cells, however, the burning cells do pressure work on other colder cells, thereby heating them through compression. Consequently, the hotter cells ignite later than those in the isolated-cells case, while the colder cells ignite earlier. This effect amounts to a modification of the ignition delay correlation Eq. (2) in two ways, in that: (a) the heat release and temperature rise no longer occur in a constant-volume mode, leading to a different pre-exponential factor (via the effective specific heat variation), and (b) local mixtures can be treated as igniting at an effective initial temperature, \( T_{0,\text{eff}} \), which is higher than \( T_0 \) due to the compression heating. The effective initial temperature is then determined by a curve fit:

\[
\frac{1}{T_{0,\text{eff}}} = \frac{1}{2T_0} \left[ 1.97 + 0.03 \tanh \left( \frac{T_0 - 1055}{25} \right) \right], \quad (3)
\]

such that \( T_{0,\text{eff}} = T_0 \) for the mixture at the highest temperature, as it is the first to ignite, and thus is not preheated by compression. For all other mixture cells, \( T_{0,\text{eff}} > T_0 \) due to compression heating prior to ignition. Using the relation for the effective initial temperature, the correlation for the ignition delay for the pressure-coupled cells is found to be

\[ \tau_{ipc} = 1.041 \times 10^{-12} \exp \left( \frac{23,000}{T_{0,\text{eff}}} \right) \text{[s]}, \quad (4) \]

which is shown as the dashed line in Fig. 1, fitting the one-dimensional calculation results very well.

In the two-dimensional turbulent ignition case, the mass and heat transport processes will affect further the ignition behavior in addition to temp-
perature and compression heating effects as shown here. Eqs. (3) and (4) thus serve as reference cases that suppress the mixing aspects from turbulent ignition, and will be used later in determining a criterion to identify the different ignition regimes.

3.2. Evolution of ignition kernels

We now investigate the two-dimensional turbulent ignition cases. Figure 2 shows two instantaneous images of the temperature field at 0.4 and 1.53 ms for Case A. During the induction period, the initial random temperature field is further deformed and dissipated by the turbulent flow. As shown in a previous study [15], local mixing and dissipation rates play an important role in determining the ignition spot among several candidate kernels. The smaller and more stretched kernels lose the race for thermal runaway, while the more aggregate kernels survive to initiate autoignition. In Fig. 2, the two kernels marked as P and Q have the highest temperatures and they are the first ones to ignite, while kernel R is subjected to higher dissipation and fails to ignite until much later time.

As a quantitative comparison, the history of the temperature and the dissipation rate of temperature are examined for the three kernels. During the ignition delay, the heat release is small, hence temperature is considered as a nearly conserved scalar variable. Therefore, in analogy with the definition in a scalar mixing layer, the scalar dissipation rate is defined as $\chi = \dot{\rho}V_\theta^2$, where $\chi$ is the thermal diffusivity and $\theta = (T - T_{0,\text{min}})/(T_{0,\text{max}} - T_{0,\text{min}})$ is the non-dimensional temperature; $T_{0,\text{max}}$ and $T_{0,\text{min}}$ are, respectively, the maximum and minimum initial temperatures in the entire domain. Figure 3 shows that, while kernels P and Q were nearly at the same temperature at $t = 0.4$ ms, kernel Q has a higher $\chi$, and consequently it lags behind P in ignition. Kernel R is subjected to an even larger value of $\chi$, and thus becomes inactive much earlier in time. The fact that the kernels Q and R are deformed into an elongated shape clearly demonstrates that these kernels are losing energy more rapidly compared to kernel P. This result confirms that the effect of mixing and diffusion must be accounted for in predicting the ignition in turbulent flows.

3.3. Effects of temperature distribution

Figure 4 shows the temporal variation of heat release rate distribution for the three cases simulated. (See Appendix A for an animation of the results.) Since the three cases ignite at different times, the four snapshots in each column are plotted at comparable times based on the fractional amount of the total heat release, at 5%, 20%, 50%, and 90%.

Case A is without the skewness in the temperature distribution and shows a baseline ignition behavior. At 5% heat release, a number of ignition kernels have developed, and thermal runaway has initiated. Once the fuel in the initial kernels is consumed, the reaction propagates into the adjacent colder mixtures in the form of reaction fronts. The heat release from the burning regions leads to compression heating of the entire domain, which subsequently triggers more hot spots that develop further into reaction fronts, while other fronts merge and are annihilated. When 90% of the heat release is complete, the extent of compression heating is sufficient to autoignite all the remaining end gases, such that additional volumetric explosion occurs to complete combustion.

In comparison, Case B has a skewed temperature distribution so that a hotter temperature core is initially present. Since the temperature is higher in the core region, the first ignition kernels develop at a much earlier time compared to Case A. Due to the mean temperature gradient generated by $T_0$ (Eq. (1)), much of the gases surrounding this first ignition spot are colder compared to Case A. As a result, the heat release during the initial period is dominantly from the fronts emanating out of the core region (see results at 20% heat release). At 50% heat release, the peripheral mixture has ignited and is rapidly reacting, while the core mixture is inactive because combustion has already occurred. The consumption of the end gases happens in a very similar way to Case A.

Finally, Case C shows a contrasting behavior. Since the inner core region is relatively cold, the ignition kernels begin to develop only in the surrounding gas region, and subsequently fronts form near the boundaries of the domain and propagate inwards. At 50% of heat release, while the hotter gases in the periphery form more kernels and react rapidly, the core region is conspicuously inactive. Towards the end, despite all the compression heating, the core region is not yet ready for volumetric explosion and is consumed slowly by front propagation, as shown at 90% heat release. These results show that even a mixture with identical total enthalpy can exhibit significantly different ignition development history depending on the temperature distribution statistics.

One of the key challenges in the HCCI engines is to achieve a smooth heat generation by introducing mixture inhomogeneities. Therefore, it is of practical interest to assess the effects of the differences in the temperature distribution on the overall heat release rate history. Figure 5 shows the temporal evolution of the volume-integrated heat release rate for the three cases. Compared to the baseline case (Case A), it is found that the heat generation in Case B (Case C) is advanced (retarded), and both Cases B and C reach a slightly lower peak heat release rate. Considering the observation in Fig. 4, the hotter core region in Case B tends to promote an earlier heat release rise by initiating a number of ignition kernels clus-
A momentary slowdown following the initial rise (during 1.7–2.0 ms) for Case B is due to the large difference in initial reactivity of the core and surrounding regions. After the core region is consumed and the fronts reach the surrounding cold gases, however, the expanding front cannot produce the same degree of compression heating as in Case A, such that the heat release rate is slowed down. Consequently, Case B exhibits the longest duration of burning and reduced peak heat release, which is desirable in HCCI engines. The “outside-in” ignition case (Case C) tends to show the opposite trend in that the heat release rise is more rapid and the burn duration is slightly reduced, except at the late stage. As shown in Fig. 4, in Case C the core gas is the last to burn by the front propagation, hence it takes a longer time compared to other cases, as indicated by the longer tail in Fig. 5.

More quantitative measures are given in Table 2, showing the timing of cumulative heat release and duration of burning based on progress in total energy release. It is of interest to note that the duration of burning in Case B is increased by more than 20%. Considering that the maximum temperatures in Cases A and B differ only by 5 K, the resulting extended burning duration is remarkable. Case C also shows a slightly increased duration compared to Case A. As discussed earlier, however, this is mainly due to the retarded burning rate towards the end of the reaction progress. This also implies that a cold core gas distribution can result in slow combustion of the end gas and may become a source of unburned hydrocarbon emissions and lower efficiency.

3.4. Role of flame fronts in overall heat release

The results revealed that ignition and heat release in a turbulent scalar field are not restricted to ignition kernels. Rather, the presence of a reaction front was evident during the ignition process. As discussed in the introduction, the reaction front can either be a spontaneous propagation front or a deflagration. While the former is a broad-range explosion driven by autoignition, the latter is a narrow reaction front whose speed depends on the transport of heat and radicals. The disparity in the length scales of these two fronts is seen in Fig. 4, where the thin flame fronts can be distinguished from the broad ignition fronts and kernels. This difference in length scales is also manifested in the magnitude of temperature gradient in the non-flame and flame zones, which vary between 300 and 5000 K/mm. This suggests that the local temperature gradient can be used as a diagnostic variable to distinguish flames from the ignition fronts. Therefore, each instantaneous solution field is divided into the two zones based on a cut-off value of the temperature gradient at 1800 K/mm. Qualitative trends were found to be consistent with different choices of the cut-off values.

Based on this criterion, the instantaneous volume fraction of the “flame-like” front and its contribution to the total heat release are compared between the three cases as shown in Fig. 6. Although the maximum heat release contribution from flame fronts was never greater than 25% for all cases, it is still a significant amount considering that the volume fraction of these regions is only around 10%. The remainder of the heat release

![Fig. 5. Comparison of volume integrated heat release rates.](image)

![Fig. 6. Fraction of heat release and volume occupied by the flame fronts.](image)

Table 2

<table>
<thead>
<tr>
<th>Case</th>
<th>Timing (ms)</th>
<th>Duration of burning (%–95%) (ms)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>5%</td>
<td>95%</td>
</tr>
<tr>
<td>A</td>
<td>1.943</td>
<td>2.837</td>
</tr>
<tr>
<td>B</td>
<td>1.745</td>
<td>2.830</td>
</tr>
<tr>
<td>C</td>
<td>1.968</td>
<td>2.921</td>
</tr>
</tbody>
</table>
is attributed to spontaneous ignition fronts and kernels. Figure 6 clearly shows that the time at which the presence of flame is prominent is shifted to earlier (Case B) and later (Case C) times in the overall ignition duration relative to that in Case A, consistent with the visual observation from Fig. 4. The ratio of the cumulative heat release from flame front to the total heat release is found to be 17.5%, 17.1%, and 13.6% for Cases A, B, and C, respectively. Case B has approximately 20% of the heat release coming from flame fronts during the initial 1ms of heat release, and its cumulative contribution is close to Case A. On the other hand, Case C has a lower contribution from flame fronts throughout the ignition process except during the last phase when the overall heat release is low. This can be explained by comparing the distribution of ignition kernels at 5% in Fig. 4. Case C has more widespread ignition kernels in close proximity than in Case A, thereby lowering the chances of flame propagation. These results demonstrate that the temperature distribution plays a crucial role in determining the importance of flames during ignition.

3.5. Ignition regimes: spontaneous versus deflagration

The above results revealed that the ignition kernels occurring in a turbulent scalar field develop into two distinct ignition regimes depending on the local mixture conditions: a wide-range spontaneous explosion and a narrow flame-like deflagration. Zeldovich [7] showed that the speed of a spontaneous ignition front is given by $S_{sp} = \left(\frac{d_s}{d_T} \cdot |VT_0|\right)^{-1}$, where $\tau_{ig}$ is the ignition delay of a homogeneous mixture at $T_0$. In the present study, the pressure-coupled case Eq. (4) is used to define $d_s/d_T$.

The above equation implies that, when the temperature gradient is low, the propagation speed can become very high compared to the laminar flame speed [8]. On the other hand, when the temperature gradient is large, instead of propagating at a vanishing speed, the reaction front transitions into a deflagration wave whose speed is controlled by the molecular transport processes. These two regimes of ignition are defined as “spontaneous propagation” and “deflagration” regimes, respectively. Following the idea of Zeldovich [7], and similar to our earlier work in a counterflow configuration [16], a criterion based on the propagation speeds of the spontaneous ignition front and deflagration wave is proposed to distinguish between the two ignition regimes. Note that the criterion based on the temperature gradient discussed in the previous section can serve as a diagnostic tool to identify the regions burning as deflagration fronts in an instantaneous solution field, whereas the present criterion is a predictive one that can determine the formation of deflagration fronts a priori based on conditions prior to the onset of ignition.

To estimate the deflagration wave speed, $S_d$, one-dimensional simulations were performed with similar initial temperature distributions [17], where the temporal variation in the front speed was monitored. The speed of the front was found to be fairly constant as the effect of non-uniform initial temperature was cancelled by compression heating. Under the fuel-lean and high-pressure condition considered in this study, a value of 50 cm/s was found to be a good estimate for the deflagration wave speed.

Based on the two characteristic speeds, $S_{sp}$ and $S_d$, a transition parameter, $\beta$, is defined as $\beta = C_\beta S_d/S_{sp}$ indicating the relative dominance of the two ignition regimes. Here, $C_\beta$ is a constant of order unity, which is chosen to be 0.5 in the present study. If $\beta < 1$, which occurs when the mixture is highly reactive and the temperature gradient is small, each local point will ignite as homogeneous explosion, and the resultant spontaneous ignition front will have a speed much higher than the deflagration speed. On the other hand, $\beta > 1$ implies that the low reactivity of the mixture will allow the deflagration front development within the mixture upon ignition. The choice of the constant, $C_\beta$, being less than unity is based on the physical consideration that there will be some delay in developing a deflagration from the ignition kernel even, if the mixture condition is ripe for the deflagration wave formation; hence, the realistic estimate for $S_d$ should be lower than the speed of a fully established flame.

The proposed criterion is applied to the solution fields at 1% heat release for the three cases, as shown in Fig. 7. The results clearly predict that a deflagration front is expected to appear with equal probability throughout the domain (Case A), or clustered in the core gas region (Cases B and C), consistent with the observation in Fig. 4. It is of interest to note that, while most of the $\beta > 1$ regions are located where the temperature gradient is large, not all the high temperature gradient regions lead to the formation of deflagration. A different choice of $C_\beta$ yields a qualitatively consistent result. This demonstrates that the parameter $\beta$ can serve as an indicator to predict the subsequent ignition behavior that may occur in one of the two different regimes. Such information can be used in developing the ignition sub-models in large-scale multi-dimensional simulation of HCCI combustion.

4. Conclusions

High fidelity simulations were performed to study the effects of different temperature distributions on the autoignition of a turbulent homogeneous mixture. In particular, the effects of hot and cold core gases on the heat release of the sys-
tem were examined. The results showed that the temperature distribution and mixing rate have a major influence on the location of the first ignition sites and the subsequent combustion and heat release. It was found that the presence of a hot core gas leads to an increase in burn duration, while a cold core gas may lead to an undesirable slow combustion of the end gas.

Based on the temperature gradient cut-off, the contribution of thin flame fronts to the total heat release was evaluated. The three cases showed distinct behavior in the dominance of the flame fronts during the duration of ignition. Finally, a predictive criterion to determine the two ignition regimes, the spontaneous propagation and the deflagration, has been defined based on the ratio of their propagation speeds. The predictions were found to be consistent with the simulation results, suggesting a potential modeling strategy for large-scale simulations of HCCI engines.

Acknowledgments

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Appendix A. Supplementary data

Supplementary data associated with this article can be found in the online version at doi:10.1016/j.proci.2004.08.176.

Comment

A.R. Masri, University of Sydney, Australia. The effects of turbulence on ignition are not straightforward. Can you comment on the possible effects that varying the initial turbulence may have on your results?

Reply. The focus of this paper was primarily on the effect of different initial temperature distributions on ignition. We have also found evidence that turbulent straining modulates the temperature gradients, and this is the topic of current investigation.