The Role of Differential Diffusion during Early Flame Kernel Development under Engine Conditions - Part II: Effect of Flame Structure and Geometry

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Abstract

From experimental spark ignition (SI) engine studies, it is known that the slow-down of early flame kernel development caused by the (Le > 1)-property of common transportation-fuel/air mixtures tends to increase cycle-to-cycle variations (CCV). To improve the fundamental understanding of the complex phenomena inside the flame structure of developing flame kernels, an engine-relevant DNS database is investigated in this work. Conclusive analyses are enabled by considering equivalent flame kernels and turbulent planar flames computed with Le > 1 and Le = 1. In Part I of the present study (Falkenstein et al., Combust. Flame, 2019), a reduced representation of the local mixture state was proposed for the purpose of this analysis. Fluctuations in heat release rate attributed to differential diffusion were found to be governed by the parameters local enthalpy, local equivalence ratio, and H-radical.

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mass fraction. Here, a coupling relation for the diffusion-controlled mixture parameter local enthalpy with local flame geometry and structure is derived, characterized by the key parameters $\kappa$ and $|\nabla c| / |\nabla c|_{\text{lam}}$. The analysis shows that the large positive global mean curvature intrinsic to the flame kernel configuration may detrimentally affect the local mixture state inside the reaction zone, particularly during the initial flame kernel development phase. External energy supply by spark ignition may effectively bridge over this critical stage, which causes the impact of global mean flame kernel curvature to be small under the present conditions compared to the overall effect of $\text{Le} \neq 1$ observed in a statistically planar flame. Once ignition effects have decayed, the mixture state inside the reaction zone locally exhibits an identical dependence on $|\nabla c|$ as in a strained laminar flame. This implies that differential diffusion effects under engine-typical Karlovitz numbers are not weakened by small-scale turbulent mixing, which is undesirable for the engine application, but can be favorable in terms of modeling.

**Keywords:** Flame Kernel, Differential Diffusion, Flame Stretch, DNS, Premixed Flame, Spark-Ignition Engine

1. **Introduction**

The reduction of cycle-to-cycle variations (CCV) in spark ignition (SI) engines is a prerequisite for the design and control of engines with increased efficiency \[2, 3\] and reduced emissions \[4, 5\]. From experiments it is well-known that CCV are correlated with the duration of flame kernel development, which was found to be sensitive to stretch effects in $\text{Le} \neq 1$ mixtures \[6\]. The development of models that capture differential diffusion effects during
early flame kernel development requires a detailed understanding of the complex parameter interactions inside the unsteady flame structure, which can be well-addressed by analysis of relevant DNS data.

A reduced representation of the governing phenomena in premixed turbulent flames is provided in Fig. 1 based on \( c \) as a synonym for a reaction progress variable, e.g. a (normalized) temperature or a quantity representative for the major product species. We begin the discussion of local effects inside the flame structure that are related to differential diffusion by considering the impact of the local reaction progress variable source term \( \dot{\omega}_c \) (cf. \( \bigcirc \) in Fig. 1), which is related to the local heat release rate. Heat release induces a flame normal propagation velocity \( s_{\text{rn}} \) and causes flow dilatation, which affects the tangential strain rate \( a_t \). These quantities enter the \((|\nabla c|\)-Eq., which additionally depends on flame curvature \( \kappa \). The local flame structure characterized by \( |\nabla c| \) in turn enters the \((\kappa)\)-Eq. (through \( s_{\text{d}} \)), which describes the evolution of local flame geometry. Obviously, the turbulent flow field plays a vital role in changing both \( |\nabla c| \) and \( \kappa \), which is here considered mainly as an external effect on the flame. For a discussion on Lewis-number-dependent feedback from the flame on the surrounding flow field, the reader is referred to the studies by Chakraborty et al. [7, 8]. The effect of the local heat release rate on the evolution of flame structure [9] and geometry [10] was investigated for different Lewis numbers, including the correlation between \( \kappa \) and \( |\nabla c| \) [11]. Coupling in the opposite direction, i.e. \( \dot{\omega}_c \)-response to changes in flame structure and geometry (cf. Fig. 1) has been mainly discussed in terms of the competition between focusing and defocusing of heat and reactants [12,14]. However, this simplified view based
on only two representative scalar fields may not be sufficient to explain all phenomena in multi-species mixtures [15, 16]. Recently, Wang et al. [17] conducted a parametric study to assess the effect of nominal equivalence ratio on heat release in high-Karlovitz H$_2$/air flames. Strong variations in heat release were observed, which correlated with local temperature and local equivalence ratio. The latter two quantities varied significantly across the reaction zone due to differential diffusion effects, particularly under ultra-lean conditions. A reaction pathway analysis revealed the influence of changed radical availability and reaction rate constants on local heat release. It should be noted that at very high Karlovitz numbers, molecular diffusion is overshadowed by small-scale turbulent mixing [18], which relaxes the local equivalence ratio (and enthalpy) towards the nominal values of the unburned mixture, i.e. both quantities may vary less in flames located in the distributed burning regime than in laminar flames [19, 20]. However, even at high-Karlovitz conditions, differential diffusion was found to be important during turbulent flame development [21, 22].

Under conventional SI engine conditions, Karlovitz numbers are actually closer to unity and differential diffusion effects substantially reduce the global heat release rate during early flame kernel development, as shown in Part I of the present study [1]. A comparative macroscopic analysis following the ($\dot{\omega}_c$)-Eq. in Fig. 1 attributed the detrimental impact of differential diffusion to the flame normal propagation velocity. A subsequent micro-scale analysis identified the governing parameters that capture the effect of turbulence on the local reaction progress variable source term $\dot{\omega}_c$. Specifically, the local mixture state that determines $\dot{\omega}_c$ was shown to be well-represented by the
local equivalence ratio $\phi$, enthalpy $h$, and the H-radical mass fraction $Y_H$.

In the present manuscript, the coupling term between the mixture state parameters and the local flame structure and geometry is exemplarily derived for the enthalpy equation in Sect. 3. The analysis presented in Sect. 4 demonstrates how the flame-kernel-intrinsic global mean curvature alters the local mixture state and heat release rate. Further, the effect of turbulence on the flame structure is shown by relating the behavior of flame kernels to strained laminar flames.

2. Summary of the DNS Database

Since the DNS database and solution methods for laminar flames have been described in Part I of the present study [1], only a brief summary of the datasets is provided hereafter. In total, four flame configurations have been computed. The main reference case is a flame kernel developing in homogeneous isotropic turbulence with fully homogeneous, stoichiometric iso-octane/air mixture and $Le > 1$. An equivalent dataset has been generated for a statistically planar flame. Additionally, both flame configurations computed in the $Le = 1$ limit [23, 29] are available for this study. The flame conditions and non-dimensional groups are listed in Tabs. 1 and 2, respectively. In Tab. 1, the mixture thermodynamic state is given by the pressure $p^{(0)}$ and temperature of the unburned gas $T_u$ with equivalence ratio $\phi_u$. Note that the turbulent flow field corresponds to decaying homogeneous isotropic turbulence, which explains the DNS parameter ranges given in Tab. 2. The turbulent integral length scale and eddy turnover time are denoted by $l_t$ and $\tau_t$, $\eta$ is the Kolmogorov length scale, while the laminar flame thickness
Figure 1: Reduced representation of turbulence/flame interactions on the integrated progress variable source term $\overline{\dot{\omega}_c}$ in presence of differential diffusion ($Le_k \neq 1$). Two analysis pathways are suggested: 1⃝ A macroscopic perspective based on the flame surface density (FSD) concept (cf. r.h.s. of $\overline{\dot{\omega}_c}$-Eq. in the blue box) considers a propagating flame front with deviations in flame displacement speed from an unstretched laminar flame, similar to laboratory experiments or classical asymptotic theories [30, 31]. 2⃝ A micro-scale perspective on the local source term $\dot{\omega}_c$, which is determined by the local mixture state, characterized by the local equivalence ratio $\phi$, enthalpy $h$, and radical mass fraction $Y_{\text{radical}}$. In case of $Le_k \neq 1$, these parameters change according to the local flame structure ($|\nabla c|$) and geometry ($\kappa$), which leads to a response in $\dot{\omega}_c$ to external perturbations of the flame, e.g. by turbulence. Note that turbulent fluctuations in the scalar fields ahead of the flame have been omitted. For more details, refer to [1].
Table 1: Flame conditions in the DNS.

| Property                | Value                      |
|-------------------------|----------------------------|
| Mixture                 | Iso-Octane/Air             |
| $p^{(0)}$               | 6 bar                     |
| $T_u$                   | 600 K                     |
| $\phi_u$                | 1.0 (homogeneous)         |
| $s_i^p$                 | 0.73 m/s                  |
| $l_f$                   | 69.1 $\mu$m               |
| Flow Field              | Decaying h.i.t.           |
| Combust. Regime         | Thin Rct. Zones           |
| $L_{\text{eff}}$        | 2.0 | 1.0 |
Table 2: Engine [32][33] and DNS characteristic numbers (Le > 1).

| Parameter | Engine   | DNS (t\textsubscript{init} - t\textsubscript{end}) |
|-----------|----------|-----------------------------------------------|
| Re\textsubscript{t} | 100 - 2390 | 385 - 222 |
| $\frac{\text{u}_{\text{rms}}}{\text{q}\textsubscript{i}}$ | 2 - 15 | 5.9 - 2.8 |
| Ka | 1 - 6 | 10.6 - 3.2 |
| Da | 1 - 100 | 1.9 - 4.6 |
| $\frac{t\textsubscript{f}}{\eta}$ | 100 -200 | 87.2 - 57.2 |
| $\frac{t\textsubscript{f}}{l\textsubscript{f}}$ | 20 - 147 | 10.9 - 13.0 |
| $\frac{D\textsubscript{0}}{l\textsubscript{f}}$ | < 1.0 | 0.3 | $\infty$ |

and initial flame diameter are referred to as $l\textsubscript{f}$ and $D\textsubscript{0}$, respectively.

A brief summary of the DNS setup is given in Tab [3]. One important difference between the flame kernel datasets and the planar reference flames is the initialization method. Flame kernels were ignited by a source term in the temperature equation, which results in an early growth phase comparable to engine experiments reported in literature as shown in [29]. By contrast, a laminar unstretched flame was imposed into the turbulent flow field as initial condition for the planar-flame DNS to avoid strong dilatation due to the larger burned volume.
Table 3: Computational setup of the DNS.

| Property                        | Value                          |
|---------------------------------|--------------------------------|
| Grid Size                       | $960^3$                        |
| Domain Size                     | $15 \cdot l_t$                 |
| Navier-Stokes Eq.               | Low-Mach-Approx. [34]           |
| Transport Model                 | Curt.-H. [35], const.-Le        |
| Soret Effect                    | yes                            |
| Chem. Mechanism                 | 26 Spec., based on [36]         |
| Flame Kernel Init.              | Ignition Heat Source            |
| Sim. Time of Flame-Kernel       | $1x \left( t_{sim.} = 3.4 \cdot \tau_t \right)$, |
| Kernel Realizations             | $3x \left( t_{sim.} = 1.0 \cdot \tau_t \right)$ |
3. Mathematical Formulation: Differential Diffusion Effects in the Enthalpy Equation

Specifically in stretched flames, differential-diffusion induces variations in element mass fractions (i.e. local equivalence ratio) \[37, 38\], enthalpy \[39\] and radical mass fractions \[15, 40, 41\] across the flame structure. Consequently, changes in chemical reaction rates and pathways may occur in presence of strong stretch \[17\]. In Part I of the present study \[1\], the combination of \((\phi, h, Y_H)\) was identified as the most suitable parameter set to capture differential-diffusion-induced variations in heat release rate conditioned on the reaction progress variable, in agreement with existing literature. Recall that in the present DNS database, the unburned mixture is fully homogeneous, i.e. variations in local enthalpy or equivalence ratio develop inside the flame structure (with the exception of the initial spark ignition in case of flame kernels). Hence, the occurrence of inhomogeneous enthalpy and equivalence ratio is mainly a diffusion-driven flame response to external changes in flame structure and geometry. In the following, the mathematical parameter relationship will be derived for the enthalpy in the planar flame dataset. Similarly, one could consider transport equations for the element mass fractions as shown by van Oijen and de Goey for a premixed counter-flow configuration \[42\], which is not pursued here for brevity. While enthalpy was not numerically solved for in the present DNS, a formula consistent with the employed transport model will be derived. We begin with the balance equation for an enthalpy variable \(h\) defined as the sum of the sensible and
chemical enthalpies \[\text{[43]},\text{ here simplified for low-Mach-number flows:}\]

\[
\frac{\partial (\rho h)}{\partial t} + \frac{\partial (\rho u_j h)}{\partial x_j} = \frac{dp^{(0)}}{dt} - \frac{\partial q_j}{\partial x_j} + \dot{S}_{\text{ign}} + \tau_{ij} \frac{\partial u_i}{\partial x_j} + \dot{q}_{\text{rad}}. \tag{1}
\]

In this work, viscous heating and radiative heat losses have been neglected.

For the present analysis, the isobaric, planar-flame DNS dataset is considered. In absence of an ignition heat source, Eq. (1) can be simplified for this specific case:

\[
\frac{\partial (\rho h)}{\partial t} + \frac{\partial (\rho u_j h)}{\partial x_j} = - \frac{\partial q_j}{\partial x_j}. \tag{2}
\]

The enthalpy flux \(q_j\) is defined as:

\[
q_j = -\lambda \frac{\partial T}{\partial x_j} + \rho \sum_{k=1}^{N_{sp}} h_k Y_k V_{j,k}
= -\rho D_{th} \frac{\partial h}{\partial x_j} + \rho \sum_{k=1}^{N_{sp}} \left[ h_k \left( Y_k V_{j,k} + D_{th} \frac{\partial Y_k}{\partial x_j} \right) \right], \tag{3}
\]

where the relation \(h = \sum (Y_k h_k)\) has been applied. Note that if a simple diffusion model of the form \(V_{j,k} = -\frac{D_{th}}{Le_k Y_k} \frac{\partial Y_k}{\partial x_j}\) was used and all species Lewis numbers were equal to unity, the last term in Eq. (3) would cancel out.

The molecular transport expressions employed in this work \[\text{[23]}\] yield a more complex net diffusion velocity:

\[
V_{j,k} = v_{j,k} + v_{jmc}
= -\frac{D_{th}}{Le_k Y_k} \frac{\partial Y_k}{\partial x_j} - \frac{D_t}{\rho Y_k T} \frac{\partial T}{\partial x_j} + \sum_{k=1}^{N_{sp}} \frac{D_{th}}{Le_n X_n} \frac{\partial X_n}{\partial x_j}. \tag{4}
\]
To obtain a form of the enthalpy equation that explicitly contains the species Lewis numbers, Eqs. (4) and (3) are combined as:

\[ q_j = - \rho D_{th} \frac{\partial h}{\partial x_j} \]

\[ - \rho D_{th} \sum_{k=1}^{N_{sp}} \left[ \left( \frac{1}{Le_k} - 1 \right) h_k \frac{\partial Y_k}{\partial x_j} \right] \]

\[ - \rho D_{th} \sum_{k=1}^{N_{sp}} \left[ \frac{1}{Le_k} Y_k h_k \frac{1}{W} \frac{\partial W}{\partial x_j} \right] \]

\[ + \rho D_{th} \sum_{k=1}^{N_{sp}} \left[ \frac{1}{Le_k} Y_k \frac{1}{X_k} \frac{\partial X_k}{\partial x_j} \right] \cdot h \]

\[- \sum_{k=1}^{N_{sp}} \left[ D_{T,k} h_k \frac{1}{T} \frac{\partial T}{\partial x_j} \right]. \quad (5)\]
Inserting this expression for the enthalpy flux into Eq. (2) yields:

\[
\frac{\partial (\rho h)}{\partial t} + \frac{\partial (\rho u_j h)}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \rho D_{th} \frac{\partial h}{\partial x_j} \right) \quad \mathcal{D}_h
\]

\[
+ \frac{\partial}{\partial x_j} \left( \rho D_{th} \sum_{k=1}^{N_{sp}} \left[ \frac{1}{Le_k} \left( \frac{1}{Le_k} - 1 \right) h_k \frac{\partial Y_k}{\partial x_j} \right] \right) \quad \mathcal{D}_{Le}
\]

\[
+ \frac{\partial}{\partial x_j} \left( \rho D_{th} \sum_{k=1}^{N_{sp}} \left[ \frac{1}{Le_k} Y_k h_k \frac{1}{W} \frac{\partial W}{\partial x_j} \right] \right) \quad \mathcal{D}_W
\]

\[
- \frac{\partial}{\partial x_j} \left( \rho D_{th} \sum_{k=1}^{N_{sp}} \left[ \frac{1}{Le_k} Y_k X_k \frac{1}{X_k} \frac{\partial X_k}{\partial x_j} \right] \right) \quad \mathcal{D}_{mc}
\]

\[
+ \frac{\partial}{\partial x_j} \left( \sum_{k=1}^{N_{sp}} \left[ D_{T,k} h_k \frac{1}{T} \frac{\partial T}{\partial x_j} \right] \right) \quad \mathcal{D}_T
\]

(6)

The first term in the r.h.s. of Eq. (6) corresponds to molecular diffusion of enthalpy and is denoted as \( \mathcal{D}_h \). Note that \( \mathcal{D}_h \) is independent of nonequal transport properties among different species. Differential diffusion may introduce local variations in enthalpy through \( \mathcal{D}_{Le} \), which vanishes in unity-Lewis-number mixtures. As will be shown below, the remaining three terms are comparatively less important in the present flame configurations, but do not cancel out in the limit of mass equidiffusion in an initially gradient-free enthalpy field. The term \( \mathcal{D}_W \) corresponds to diffusion due to spatial variations in molecular weight and \( \mathcal{D}_T \) represents thermodiffusion. Since the applied diffusion model requires a correction term to enforce mass conserva-
tion, the associated enthalpy transport appears as $D_{mc}$ in Eq. (6). All terms have been evaluated in the planar DNS dataset with $Le \neq 1$. The results shown in Fig. 2 confirm that the differential diffusion term $D_{Le}$ is of leading order. It is balanced by molecular diffusion of enthalpy through $D_{h}$. In order to further investigate the role of differential diffusion in the present turbulent flames, we seek to identify the governing flame parameters which are suitable for conditional averaging of the DNS results and enable a rigorous comparison to laminar reference solutions.

After splitting the species mass diffusion terms into components by normal- and tangential diffusion [14], the differential diffusion term $D_{Le}$ in Eq. (6) can be rewritten in terms of the scalar-iso-surface curvature $k(Y_k)$ and the scalar-
gradient magnitude $|\nabla Y_k|$: 

$$D_{Le} = \sum_{k=1}^{N_{sp}} \frac{\partial}{\partial x_j} \left( \rho D_{th} \left( \frac{1}{Le_k} - 1 \right) h_k \frac{\partial Y_k}{\partial x_j} \right)$$

$$= -\sum_{k=1}^{N_{sp}} \left( \rho D_{th} \left( \frac{1}{Le_k} - 1 \right) h_k |\nabla Y_k| \kappa(Y_k) \right)$$

$$- \sum_{k=1}^{N_{sp}} \frac{\partial}{\partial x_{n,k}} \left( \rho D_{th} \left( \frac{1}{Le_k} - 1 \right) h_k |\nabla Y_k| \right)$$

(7)

It should be noted that in this work, the curvature $\kappa$ of iso-surfaces belonging to any scalar field $\vartheta$ is computed from the normal vector $n_i$ pointing into the direction of negative scalar gradient, i.e. flame kernels have positive global mean curvature:

$$\kappa^{(\vartheta)} = \frac{\partial n^{(\vartheta)}_i}{\partial x_i},$$

$$n^{(\vartheta)}_i = \frac{-1}{|\nabla \vartheta|} \frac{\partial \vartheta}{\partial x_i}.$$  

(8)

(9)

To parameterize differential diffusion under the present engine-relevant DNS conditions, the turbulent scalar field shall be related to the laminar unstretched flame in points where $|\nabla Y_k|_{\text{lam}} > 0$. Further, we assume that

$$\kappa^{(Y_k)} \approx \kappa^{(T)},$$

$$\frac{|\nabla Y_k|}{|\nabla Y_k|_{\text{lam}}} \approx \frac{|\nabla T|}{|\nabla T|_{\text{lam}}},$$

(10)

(11)

i.e. scalar iso-surfaces are considered to be parallel and scalar gradients inside the flame structure are proportionally compressed or expanded if the local flame thickness deviates from the unstretched premixed flame. Introducing these assumptions into Eq. (7) yields the approximate differential diffusion
As will be shown below, using $\kappa$ as a measure for local flame geometry and $|\nabla \vartheta|/|\nabla \vartheta|_{\text{lam}}$ for a representative scalar $\vartheta$ to characterize changes in flame structure with respect to a laminar reference flame works reasonably well to parameterize differential diffusion under the present engine-relevant DNS conditions. It can be expected that in presence of strong turbulent micro-mixing, the applied analogy to a laminar reference flame does not hold.

To demonstrate that the assumptions (10) and (11) hold on average under the present conditions, both parameters have been evaluated from different species and based on temperature. Conditional mean results are plotted as function of the temperature-based quantities in Fig. 3. Note that the data has been conditioned on non-zero scalar gradients to avoid singularities, but not on specific temperature iso-levels. The strong correlation between flame curvatures computed from different quantities (cf. Fig. 3(a)) confirms the assumption that scalar iso-surfaces in the same spatial location are mostly parallel to each other. Similarly, the correlation between scalar-gradient ratios is shown in Fig. 3(b). The respective laminar reference gradient is mapped based on the local temperature value. Although the correlation with the temperature-based parameter is less strong compared to the curvature results, the conditional mean gradient ratios evaluated for different species scatter around the diagonal, which is sufficient for the present analysis.
In this section, the mathematical relation between the local mixture state (which determines $\dot{\omega}_c$) and flame structure and geometry has been derived. Eq. (12) suggests the following hypothesis for turbulent premixed flames with Karlovitz numbers not much higher than unity: differential diffusion effects approach the limit of a laminar unstretched flame, if the curvature is zero and the local temperature gradient is comparable to the laminar reference flame. This hypothesis and the actual quantitative effects of differential diffusion in both the planar-flame and the engine-relevant flame kernel configuration will be discussed below.

4. Results

Since differential diffusion introduces a strong coupling between the local mixture state and the flame geometry and structure (cf. (D$_{Le}$)-Eq. in Fig. 1), the particular conditions during early flame kernel development require special attention. In Sect. 4.1, differences between the flame kernel and the planar flame configuration that can be attributed to curvature effects will
be investigated. The role of turbulence in changing the flame structure will be analyzed in Sect. 4.2 by relating the behavior of flame kernels to laminar flame solutions.

4.1. Combined Effect of Flame Geometry and Structure

In Part I of this study [1] it was shown that the mean heat release rate conditioned on the reaction progress variable (temperature) is significantly reduced by differential diffusion effects in the present flames with \( \text{Le} > 1 \). Further, the local mixture state at a given progress variable was shown to be well-represented by the reduced parameter set \((h, \phi, Y_H)\). Here, the difference between the flame kernel configuration that features positive global mean curvature due to the quasi-spherical flame shape and the planar flame configuration will be analyzed. To this end, the evolution of the governing parameters inside the flame structure of flame kernels will be considered in a first step.

In Fig. 4 the overall impact of differential diffusion is shown by the results extracted from the fully-developed planar flames computed with \( \text{Le} > 1 \) and \( \text{Le} = 1 \). In addition, results for flame kernels with \( \text{Le} > 1 \) are shown. For a spherical expanding flame with \( \text{Le} > 1 \) and substantial mean curvature, one would expect a stronger reduction in heat release rate with respect to the laminar unstretched limit than in case of a statistically planar flame, which is confirmed by the flame kernel results extracted at \( t = 1.92 \tau_l \) (cf. Fig. 4(a)). At this time instant, compared to the corresponding planar flame dataset, the mixture state inside the reaction zone (indicated by the two vertical lines) is characterized by reduced levels of both \( h \) and \( \phi \), as well as a lower peak H-radical fraction. During the very early phase of flame kernel
Figure 4: Effect of differential diffusion on conditional mean heat release rate (a) enthalpy (b), local equivalence ratio (c) and H-radical mass fraction (d) as function of temperature for the planar flames and the $\text{Le} > 1$ flame kernel configuration. The vertical lines indicate the $\text{H}_2$-consumption layer \cite{36}. For the flame kernel results, the earlier two times are computed with four realizations, the last time with only one.

development, the detrimental effect of differential diffusion on the heat release rate is effectively compensated by spark ignition, which leads to an increased enthalpy level inside the flame structure (cf. Fig. 4(b)).

Since mean flame curvature is an intrinsic property of the flame kernel configuration, we will now focus on the flame response to local curvature, and use the findings to estimate the effect of global mean flame curvature on the heat release rate of flame kernels afterwards. According to Eq. (12), differential-diffusion-induced variations in enthalpy across the flame struc-
ture depend on both the local curvature and a representative scalar gradient. Although $\kappa$ is not explicitly contained in the second term in the r.h.s. of Eq. (12), the occurrence of curvature will typically alter both terms due to the coupling between $\kappa$ and $|\nabla c|$ in premixed flames (cf. (\(\kappa\))- and $(|\nabla c|)$-Eqs. in Fig. 1). To assess the development of the flame structure of the expanding flame kernels after spark ignition, the mean temperature gradient conditioned on curvature has been evaluated for the temperature iso-surface corresponding to the maximum heat release rate in an unstretched premixed flame ('$T_{\text{maxHR}}$'). The correlations shown in Fig. 5 are overall very consistent with the Le > 1 results by Chakraborty and Cant [11]. For positive curvatures, all flames exhibit a monotonously decreasing trend. Hence, flame kernels that feature mean positive curvature will on average have lower temperature gradients compared to the planar flame. With respect to the spark effect it can be concluded that the initially high gradients decay until $t = 0.91 \tau_t$ on the entire $T_{\text{maxHR}}$-iso-surface under the present conditions. It should be noted that in the limit of zero local curvature, the temperature gradient of the turbulent flames is reduced compared to an unstretched laminar flame. This effect will be attributed to hydrodynamic strain later on. Keeping the negative correlation between $|\nabla T|$ and $\kappa$ in mind, the combined effect of externally invoked changes in flame geometry ($\kappa$) and structure ($|\nabla T|$) on the local mixture state ($h, \phi, Y_H$) and heat release rate will be analyzed in the next section.

Results for the fully developed planar flames are depicted in Fig. 6. While the curvature-conditioned mean heat release rates shown in Fig. 6(a) recover similar levels as the corresponding laminar unstretched flames in regions
with strong negative curvature ($\kappa < -1/l_f$), differential diffusion leads to a pronounced negative correlation between curvature and the chemical source term in flame regions with moderately negative as well as positive curvature. This characteristic behavior of $\text{Le} > 1$ flames has very strong negative consequences for the heat release rate of flame kernels with positive global mean curvature, which will be quantified below. Note that in the planar turbulent flame with $\text{Le} > 1$, even flame regions with zero curvature exhibit detrimental behavior in terms of the desirable high burning rate for engine applications. This reduction in heat release rate compared to a laminar unstretched flame is due to the presence of hydrodynamic strain, which is indicated in Fig. 6(a) by the laminar data point extracted from a back-to-back counterflow flame (c.f.f.) solution. The strained laminar flame solution has been selected based on the condition $|\nabla T|_{\text{maxHR,cff}} = \langle |\nabla T| \mid (T = T_{\text{maxHR}}, \kappa = 0) \rangle$ and will be analyzed in more detail in Sect. 4.2 (also refer to Fig. S-1 in the supp. material). In both the laminar strained as well as the turbulent flame, the reduction in heat release rate can be explained by the differential-
diffusion-induced decrease in enthalpy and equivalence ratio compared to the laminar unstretched limit (cf. Fig. 6(b)), i.e. by the second term in Eq. (12). Recall that the transport equations of both quantities do not have a chemical source term (cf. Eq. (6)), but there is a coupling with the heat release rate through the $\left(\left|\nabla T\right|\right)$-Eq. as shown in Fig. 1. The reduction in $Y_H$ shown in Fig. 6(b) is another causal effect for lowering the heat release rate at the considered iso-temperature level $T_{\text{maxHR}}$. However, the quantitative relation between $\dot{\omega}T|T$ and the parameters $(h, \phi, Y_H)$, which were found to well-parametrize the heat release rate across the entire flame structure (cf. Part I [1]), shows that the influence of the H-radical mass fraction is much lower than that of $h$ and $\phi$ (cf. Fig. S-2 of the supp. material). With respect to the curvature PDFs plotted in Fig. 6 (PDF$_{\Sigma|T}$: surface-weighted PDF, conditioned on $T = T_{\text{maxHR}}$), differential diffusion is shown to cause a distribution with shorter tails in the engine-relevant, $Le > 1$ case, consistent with the analysis by Alqallaf et al. [10]. Between the 10th and 90th percentile of the $Le > 1$ curvature distribution, the normalized enthalpy and local equivalence ratio vary in the ranges $h/h_{\text{lam}} = 0.97...0.63$ and $\phi = 1.05...0.81$, which are strong deviations from the $Le = 1$ limit with $h/h_{\text{lam}} \approx 1$ and $\phi \approx 1$. Since the key difference between the considered planar flames and the engine-relevant flame kernel configuration is the curvature distribution, the effect on the mean heat release rate will be estimated in the following.

The curvature distribution of flame kernels exhibits positive mean curvature, which is expected to reduce the mean heat release rate due to differential diffusion effects (cf. Fig. 6(a)). Further, the very early phase of flame kernel development is characterized by the occurrence of skewness towards high
Since positive curvature, which has been previously shown in the $Le = 1$ limit \[20\] and is confirmed in Fig. S-3 of the supplementary material for the present $Le > 1$ datasets. To investigate the impact of the curvature distribution, we have convoluted the curvature-conditioned mean heat release rate of the fully developed planar flame that was shown in Fig. 6(a) with three different curvature distributions: i) the actual curvature PDF of the $Le > 1$ flame kernel configuration (four realizations), ii) the time-varying curvature PDF of the planar flame (to assess the effect of the kernel’s mean positive curvature), and iii) an artificial curvature PDF generated from the PDF of the planar flame, but shifted to the same mean curvature as the flame kernel and renormalized (to test the effect of positive curvature skewness). This procedure has been repeated for a sequence of time instances during early flame development, while keeping the conditional mean heat release rate constant. Hence, the effect of mean curvature intrinsic to the flame kernel configuration on the mean heat release rate can be separated from differences in curvature PDF.
shape and spark effects. Additionally, this approach may be a first estimate for the performance of an ideal model designed for a fully developed flame, when applied to the flame kernel configuration. The resulting mean heat release rates on the $T_{\text{maxHR}}$-iso-surface are shown in Fig. 7 as function of time. According to this estimate, mean curvature may have a significant effect on the mean heat release rate during the very early phase of flame kernel development. However, it was shown in Fig. 4(a) that spark ignition initially leads to a higher heat release rate than in the planar flame, which is not accounted for in Fig. 7. This means that the initially strong detrimental effect of differential diffusion induced by high positive mean curvature of flame kernels (cf. Fig. 7) is effectively compensated by external enthalpy supply under the present conditions. After a time of $t \approx 0.5 \tau_1$ is reached, the reduction compared to the developing planar flame amounts to approximately 10%. Since the same applies for the planar-shifted PDF convolution, this reduction is only the effect of mean curvature of the kernel and the positive curvature skewness has only a minor effect. Also note that after $t \approx 0.5 \tau_1$, the relative difference in mean heat release rate between the flame kernel and the planar flame estimated in Fig. 7 and observed at $T_{\text{maxHR}}$ in Fig. 4(a) are very similar, which supports the validity of the preceding analysis.

Hence, it can be concluded that compared to the overall effect of differential diffusion reflected by the difference between the $\text{Le} > 1/\text{Le} = 1$ planar-flame results in Fig. 4(a), the additional reduction in mean heat release rate due to to positive mean curvature of flame kernels is rather small, thanks to initial ignition energy supply. It should also be noted that the minor influence of the PDF-shape on the mean heat release rate does not imply that charac-
Figure 7: Convolution of different time-varying curvature distributions with the conditional mean heat release rate of a fully developed turbulent planar flame with $Le > 1$ (cf. Fig. 6(a)). Data has been conditioned on $T_{\text{maxHR}}$.

4.2. Dependence of $(h, \phi, Y_{H})$ on Local Variations in Flame Structure for a given Curvature

According to Fig. 1, the local heat release rate is determined by the local mixture state, characterized by the parameter set $(c, h, \phi, Y_{H})$. For $Le_k \neq 1$, $h$ has been shown to be coupled to the local flame structure ($|\nabla c|$) and geometry ($\kappa$) through the $(D_{Le})$-term in the enthalpy transport equation (cf. Eq. (12)). While the role of flame curvature has been already discussed in Sect. 4.1, the objective here is to quantify the effect of externally invoked changes in $|\nabla c|$ due to hydrodynamic strain (cf. $(|\nabla c|)$-Eq. in Fig. 1). In the limit of $\kappa = 0$, this analysis can be consistently applied to turbulent flames and the laminar counterflow flame (c.f.f.) configuration, which has been
already used as a reference solution in Fig. 6. In the following sections, we will first show how the planar flame compares to the laminar counterflow configuration and relate flame kernel development to the fully developed planar results afterwards. For clarity, the analysis will be limited to the $T_{\text{maxHR}}$-iso-surfaces.

In Fig. 8, the flame structure of both turbulent and laminar flames is parameterized by $|\nabla T|$, which is analogous to employing the scalar dissipation rate $\chi_T$ for modeling purposes [48]. It is shown that in the fully developed planar flame with $\text{Le} > 1$, local regions with zero curvature on average exhibit $\dot{\omega}_T$ and $(h, \phi, Y_H)$ dependencies on $|\nabla T|$ that are almost identical to the laminar premixed counterflow configuration. If differential diffusion effects were significantly reduced by small-scale turbulent mixing, the effective Lewis numbers would be closer to unity [20], i.e. the slope of the conditional means would approach the plotted $\text{Le} = 1$ results. This is an important finding since the Karlovitz numbers in the present datasets are located in the upper range of conventional SI engine conditions. Note that the behavior of an unstretched laminar flame is locally recovered for $|\nabla T| = |\nabla T|_{\text{lam}}$, which confirms the chosen parametrization derived from the $(\mathfrak{D}_{\text{Le}})$-Eq. The unconditional mean value plotted as open square symbol at $|\nabla T| / |\nabla T|_{\text{lam}} \approx 0.7$ in each subfigure marks the unfavorable conditions found on average near $T_{\text{maxHR}}$-iso-surface elements with $\kappa = 0$ (also cf. Fig. 6). As a remark to the shown correlations for a constant iso-temperature, it should be mentioned that each quantity may respond to strain by changes in the overall magnitude, or by qualitatively changing its distribution across the flame structure towards lower/higher temperatures (cf. Fig. S-1 in the supp. material).
Regarding the conditional $|\nabla T|$-PDFs (PDF$_{\Sigma|T,\kappa}$: surface-weighted PDF, conditioned on $T = T_{\text{maxHR}}$ and $\kappa = 0$) shown in Fig. 8, large variance can be observed in the Le $> 1$ flame, besides the significantly reduced mean value compared to the Le $= 1$ dataset. The large variance can be explained by the strong coupling between flame structure and geometry with the local mixture state by differential diffusion as sketched in Fig. 1. Any change in scalar gradients may trigger changes in enthalpy and local equivalence ratio (cf. ($\mathcal{D}_{\text{Le}}$)-Eq.), which cause direct response in heat release rate. Since scalar gradient production depends on dilatation through the tangential strain term (cf. ($|\nabla c|$)-Eq.), a wider gradient distribution can be expected in Le $\neq 1$ flames. In the Le $= 1$ limit, external changes in $|\nabla T|$ or $\kappa$ trigger only minor variations in the local mixture state due to the Soret effect since the ($\mathcal{D}_{\text{Le}}$)-Eq. vanishes.

Now that relationships between the canonical configuration of a fully developed turbulent planar flame and strained laminar flame characteristics have been established, we seek to connect early flame kernel development to the planar-flame results. Recall that in contrast to the afore-discussed planar flames, flame kernels were ignited with a volumetric heat source of spherical shape, which provides excess enthalpy (cf. Fig. 4(b)) and high scalar gradients (cf. Fig. 5). In Fig. 9, mean enthalpy and equivalence ratio conditioned on $|\nabla T|$ are shown for three different time instances of flame kernel development. As before, the data has been conditioned on ($T_{\text{maxHR}}$)-iso-surface elements. Here, the data has been conditioned on the respective flame-averaged curvature $\langle \kappa \rangle$, i.e. for the planar flame the same data as in Fig. 8 is shown due to $\langle \kappa \rangle = 0$. At $t = 0.37 \tau_t$, excess enthalpy is available in the reaction zone.
Figure 8: Planar Flame: Conditional mean heat release rate (a), enthalpy (b), local equivalence ratio (c) and H-radical mass fraction (d) as function of normalized gradient. Data has been conditioned on $T_{maxHR}$ and $\kappa = 0$. 

\[ \frac{\langle \dot{\omega}_{maxHR,\kappa=0} \rangle}{\dot{\omega}_{lam}} \] 

\[ \frac{\langle \dot{h}_{maxHR,\kappa=0} \rangle}{\dot{h}_{lam}} \] 

\[ \frac{\langle \phi_{maxHR,\kappa=0} \rangle}{\phi_{lam}} \] 

\[ \frac{\langle Y_{H,maxHR,\kappa=0} \rangle}{Y_{H,\text{lam}}} \]
due to spark ignition (cf. Fig. 9(a)), which pushes the $|\nabla T|$-PDF towards higher mean values, despite the already lean mixture composition caused by differential diffusion (cf. Fig. 9(b)). At $t = 0.91 \tau_t$, the correlations with $|\nabla T|$ are overall fairly similar to the developed planar flame. However, the gradient distribution indicates generally reduced gradients, which is due to the presence of mean flame curvature (cf. Fig. 5). At $t = 1.92 \tau_t$, a tendency towards the gradient distribution of the developed flame can be observed, but still with significantly higher probability of low gradients. In summary, the $Le > 1$ flame kernels approach very similar conditional dependencies as the planar turbulent and strained laminar flames, after the initial non-equilibrium correlation between $\kappa$ and $|\nabla T|$ imposed by spark ignition has decayed within less than two laminar flame times. Differences between the iso-surface averaged quantities in the flame kernel and the planar flame configuration can be attributed to the overall larger flame thickness caused by the positive mean flame kernel curvature. The presented results for enthalpy and equivalence ratio are supported by similar conclusions with respect to H-radical availability shown in Fig. S-4 of the supplementary material.

Conclusions

Since experimental SI engine studies have provided evidence that differential diffusion effects in fuel/air mixtures with $Le > 1$ lead to an increase in CCV, it is desirable to assess the impact already during engine design. To enable the development of models that capture such fuel effects on CCV, the intention of the present work is to improve the understanding of the complex phenomena inside the flame structure during early flame kernel development.
To this end, a DNS database designed to be representative for engine part-load conditions has been analyzed in detail according to a suitable expression for the coupling between the local mixture state and the flame geometry and structure. Flame kernel results have been related to canonical turbulent and laminar flame configurations to enhance generality and increase the relevance of the present findings for future modeling efforts. Specifically, the following conclusions can be drawn:

- The key mathematical expression that characterizes differential diffusion effects under the present engine-relevant conditions is Eq. (12). If non-zero, this term leads to a two-way coupling between the local heat release rate and the flame geometry expressed by curvature, and flame structure expressed by a scalar gradient magnitude. In the limit of $\text{Le} = 1$, the local mixture state is barely affected by flame geometry and structure since $\mathcal{Q}_{\text{Le}} = 0$, i.e. there is mainly a one-way coupling.
from the heat release rate to scalar gradients and curvature. The substantially larger number of involved diffusive and hydrodynamic time and length scales may explain the excessive variance in heat release rate associated with the two-way-coupled system [1]. Further, the (DLe)-Eq. suggests two flame parameters for the analysis of differential diffusion effects, $\kappa$ and $|\nabla T| / |\nabla T|_{\text{lam}}$.

- It has been shown that the global mean curvature of flame kernels reduces the mixture state parameters $(h, \phi, Y_H)$ inside the reaction zone, which lowers the heat release rate and scalar gradients. This effect is most pronounced during the initial phase of flame kernel development and can therefore be effectively compensated by ignition energy supply. After ignition effects have decayed, the effect of mean kernel curvature turned out to be small compared to the overall reduction in heat release rate due to $\text{Le} > 1$ observed in a statistically planar flame (under the present conditions). However, the effect of global mean curvature is dominant over the impact of the characteristic curvature PDF shape caused by early flame kernel/turbulence interactions [29].

- As suggested by the (DLe)-Eq., in case of $\kappa = 0$ and $|\nabla T| = |\nabla T|_{\text{lam}}$, the turbulent flames should locally recover the behavior of an unstretched laminar flame. This has been confirmed by $\dot{\omega}_T$ and $(h, \phi, Y_H)$ dependencies on $|\nabla T|$ that are almost identical to the laminar premixed counterflow configuration. Hence, the significant reduction in heat release rate locally observed in turbulent flame elements with $\kappa = 0$ can be attributed to the effect of hydrodynamic strain impacting the scalar
gradient magnitude distribution. It seems that differential diffusion effects are not weakened by turbulent micro-mixing under the present engine-relevant conditions.

- The presented parameter correlations for the flame structure of flame kernels overall recover the behavior of the fully developed turbulent planar flame, after the excess enthalpy and high scalar gradients introduced by spark ignition have decayed within approximately two laminar flame times (under the present conditions).

It should be noted that the overall detrimental behavior of the stoichiometric iso-octane/air flames compared to the \( \text{Le} = 1 \) reference flames presented in this work directly translates to common transportation fuels which feature Lewis numbers larger than unity. Although the Reynolds number in the present DNS database is at least two times smaller than in practical engines, the main conclusions should remain valid under more realistic conditions since the Karlovitz number has been closely matched (cf. Tab. 2). More detailed investigations on the microscopic role of spark ignition during early flame kernel development are suggested for future work.

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