Numerical investigation of the effect of pressure on heat release rate in *iso*-octane premixed turbulent flames under conditions relevant to SI engines

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Abstract

A series of direct numerical simulations (DNS) of *iso*-octane/air turbulent premixed flames in the thin reaction zones regime have been performed in order to investigate the effect of pressure on heat release rate under conditions relevant to spark-ignition (SI) engines (up to 20 bar and 800 K in the unburnt gas). Chemistry is represented by a reduced kinetics mechanism containing 74 species and 976 reactions (reduced from CaltechMech). The effect of pressure has been isolated by fixing the Karlovitz numbers, the Lewis numbers, and the ratio of integral length scale to laminar flame thickness. On one hand, the results suggest that pressure has very limited effect on the mean heat release rate, such that turbulent burning velocity is proportional to the turbulent surface area. In addition, while the chemical pathways are strongly affected by pressure in laminar flames, the global effect of turbulence on these pathways is negligible, independent of pressure. On the other hand, the local distribution of heat release rate was found to be significantly affected by pressure through differential diffusion-chemistry effects.

Keywords: turbulent premixed flame, high pressure, *iso*-octane, thin reaction zones regime, spark-ignition engine

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1. Introduction

Turbulent premixed combustion in spark-ignition (SI) engines takes place under high pressure conditions. In typical SI engines, pressure ranges from 10 to 40 bar during most of the flame propagation.

The effects of pressure on turbulent burning velocity have been extensively investigated experimentally, over a similar range of pressures, by several authors, including [1–4]. In all these studies, the most striking observation is that turbulent burning velocity increases with increased pressure. For turbulence intensities sufficiently large that Darrieus-Landau instabilities are negligible, this increased burning velocity has been attributed to an increase in flame surface area due to small scale wrinkling [2, 5–7]. As kinematic viscosity decreases due to increased pressure, smaller turbulent structures appear. Since the laminar flame thickness also decreases with increasing pressure, the combined effect is a wrinkling of the flame front over a wider range of scales, thus increasing the turbulent flame surface area. It is important to note that in these studies the velocity fluctuations and the integral length scale were found to be weakly dependent on pressure.

All of these studies were conducted for flames in the corrugated or wrinkled flamelet regimes. While such flames can be relevant to SI engines under certain operating conditions, Linse *et al.*[8] have shown that in turbo-charged direct injection SI engines, combustion takes place in the thin reaction zones regime over a wide range of operating

Fig. 1: Schematic diagram of the flow configuration.

conditions. This regime of combustion is particularly relevant to modern engines that use high levels of exhaust gas recirculation [9, 10].

Using direct numerical simulations (DNS), several studies have shown that, in this regime, heat release rate (HRR) can be significantly affected by turbulence [11–15]. However, these simulations were performed with atmospheric pressure and, to the best of the authors’ knowledge, there is no numerical investigation in the literature of the effect of background pressure on HRR in turbulent premixed flames in the thin reaction zones regime.

The objective of this work is to investigate the effect of pressure, as an independent parameter, on HRR in turbulent premixed flames under conditions relevant to SI engines. As such, a series of DNS of *iso*-octane/air turbulent premixed flames in the thin reaction zones regime are performed with detailed chemistry. The Karlovitz numbers, the Lewis numbers, and the ratio of integral length scale to flame thickness are kept constant to isolate the effect of pressure from that of these other controlling parameters. The focus is put on statistics of the global and local HRR and the effect of turbulence on global chemical pathways, quantities which cannot be obtained from experiments.

Due to the inherent computational cost associated with high-Karlovitz DNS, only a small fraction of a realistic flame surface could be simulated. We expect that such small domain is still adequate for the purpose of the present work, which studies the effect of small scale turbulence on HRR [16].

2. Numerical approach

The numerical approach, reviewed here, follows that of Ref [13–15].

2.1. Flow configuration

Figure 1 presents a schematic diagram of the flow configuration. A statistically-planar, freely-propagating flame was chosen in order to isolate the effects of turbulence on the flame from mean flow shear and curvature effects.

Periodic boundary conditions in both the y - and z -directions and inflow/outflow in the x -direction are used. The unburnt gas is injected at constant bulk velocity with a low turbulent kinetic energy (TKE), such that there

are no negative inlet velocities. This inflow is generated from a separate homogeneous isotropic turbulence (HIT) simulation [17, 18]. Away from the inflow and outflow regions, velocity field forcing (described in Section 2.4) maintains a constant TKE across the flame. A long domain is used to avoid negative outflow velocities (decaying turbulence), to allow the flame to slightly drift, and to reach HIT both upstream and downstream of the flame (allowing the study of the effect of the flame on turbulence, such as in Bobbitt *et al.* [19]).

The simulations were run until a statistically steady state was reached. As a result, the first 15 eddy turnover times were ignored and the data were collected over at least the next 30 turnover times.

2.2. Governing equations

The low Mach number Navier-Stokes equations are used

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0, \quad (1)$$

$$\frac{\partial}{\partial t} (\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) = -\nabla p + \nabla \cdot \boldsymbol{\sigma} + \mathbf{f}, \quad (2)$$

$$\frac{\partial}{\partial t} (\rho Y_i) + \nabla \cdot (\rho \mathbf{u} Y_i) = -\nabla \cdot \mathbf{j}_i + \dot{\omega}_i, \quad (3)$$

$$\begin{aligned} \frac{\partial}{\partial t} (\rho T) + \nabla \cdot (\rho \mathbf{u} T) &= \nabla \cdot (\rho \alpha \nabla T) + \dot{\omega}_T \\ &- \frac{1}{c_p} \sum_i c_{p,i} \mathbf{j}_i \cdot \nabla T + \frac{\rho \alpha}{c_p} \nabla c_p \cdot \nabla T, \end{aligned} \quad (4)$$

where ρ is the mixture density, $\mathbf{u}$ is the velocity, p is the hydrodynamic pressure, $\boldsymbol{\sigma}$ is the viscous stress tensor, $\mathbf{f}$ is the turbulence forcing term (described in Section 2.4), Y_i is the species mass fraction, $\dot{\omega}_i$ is the species production rate, T is the temperature, $c_{p,i}$ is the species heat capacity, c_p is the mixture heat capacity, α is the mixture thermal diffusivity, and $\dot{\omega}_T$ is the temperature production term. The species diffusion mass flux, $\mathbf{j}_i$, is expressed as

$$\mathbf{j}_i = -\rho D_i \frac{Y_i}{X_i} \nabla X_i - \rho Y_i \mathbf{u}_c, \quad (5)$$

where X_i is the species mole fraction and D_i is the species diffusivity. The correction velocity $\mathbf{u}_c$ is present to ensure zero net diffusion mass flux [20]. Finally, the equation of state for a mixture of perfect gases is considered

$$\rho = \frac{P_0 W}{RT}, \quad (6)$$

where P_0 is the thermodynamic pressure, R is the universal gas constant, and W is the mixture molar weight.

Equations 1 to 6 are solved numerically using the energy conservative, finite difference code NGA [21]. The scheme selected is second-order accurate in both space (centered discrete operators) and time. A semi-implicit Crank-Nicolson time integration is used [22]. Third-order BQUICK [23] is used as the scalar transport scheme.

2.3. Chemistry and transport properties

The chemical kinetics mechanism used in the simulations corresponds to CaltechMech [24] from which the soot and linear alkane decomposition pathways have been removed. This reduced chemical model contains 74 species and 976 elementary reactions (forward and backward rates counted separately). CaltechMech has been previously validated for *iso*-octane over a wide range of unburnt temperatures and background pressures up to 25 bars (supplemental material).

The mixture viscosity and thermal diffusivity are computed as in Ref. [13–15]. In order to isolate the effects of pressure from those of differential diffusion, the species diffusivities are computed as $D_i = \alpha/Le_i$, with the Lewis numbers Le_i kept constant throughout the flame. The latter are extracted from the simulation of a one-dimensional, laminar premixed flame with full transport properties, using FlameMaster [25]. They are evaluated in the burnt gas such that deviations from the full transport solution are negligible. A single set of Lewis numbers is used for all the simulations. The Lewis number of the fuel, *iso*-octane, is $Le_F = 2.5$. As previously observed in the literature (*e.g.* [3] for pressures up to 15 bars), pressure was found to have a very limited effect on the species Lewis numbers. Assessing the effect of using a more complete diffusion model should be the subject of future work, especially if higher pressures (*e.g.* more than 50 bars) are considered [26].

2.4. Turbulence forcing

Since the flow configuration lacks generation of turbulence due to large scale flow straining, turbulence forcing is necessary [12, 27, 28]. The linear velocity forcing method [17, 29, 30] was chosen for its physical nature and good stability properties [18].

The forcing term $\mathbf{f}$ in Eq. 2 takes the following form:

$$\begin{aligned} \mathbf{f}(x, y, z, t) = & A \frac{k_0}{k(x, t)} \\ & \times (\rho(x, y, z, t) \mathbf{u}(x, y, z, t) - \overline{\rho \mathbf{u}}(x, t)), \end{aligned} \quad (7)$$

where $A = \epsilon_0/(2k_0)$ is the forcing coefficient (computed as $A = (2/27)^{1/2} (k_0/l^2)^{1/2}$ [18]), k_0 is the desired

TKE, ϵ_0 is the corresponding desired dissipation rate, and k is the planar Favre-averaged TKE. The forcing method imposes a TKE and an integral length scale l approximately constant across the flame [19], with $l = 0.19L$. This was observed in the slot burner flames of Sankaran *et al.* [31] where turbulence is generated through intense mean shear. Unfortunately, to the best of the authors' knowledge, there is no similar evidence for the present configuration (no mean shear) at high Ka . The assumption of constant TKE should be verified in future high- Re , high- Ka experimental or numerical work. Note that, independent of the forcing, baroclinic torque and dilatation were shown to have a negligible effect on enstrophy transport in similar $Le_F > 1$, high- Ka flames [19, 32].

2.5. Simulation parameters

Four simulations are performed, for which the parameters are listed in Table 1. The equivalence ratio ϕ is fixed so that the *iso*-octane/air mixture is near stoichiometry (slightly lean).

Case	P1T3	P1T3'	P20T3	P20T8
Fuel	<i>i</i> -C ₈ H ₁₈			
ϕ	0.9			
T_u (K)	298	298	298	800
P_0 (bar)	1	1	20	20
S_L (m/s)	0.32	0.32	0.11	0.93
l_F (mm)	0.40	0.40	0.045	0.021
u'/S_L	7.6	19	20	3.7
l/l_F	1.0			
Ka_u	61	234	234	16
Ka_δ	1.9	7.3	1.9	1.9
$Re_{t,u}$	65	159	140	18
$Re_{t,\delta}$	5.1	12.4	8.7	5.7
η_u (μm)	17	8.8	1.2	2.4
Δx (μm)	16	16	2.0	0.88
Domain	$11L \times L \times L$			
Grid	11×128^3			
T_{peak}^F (K)	1285	1285	1488	1550
T_{peak}^T (K)	1631	1631	1828	1976

Table 1: Simulation parameters. $Re_{t,u} = u'l/\nu_u$, $Re_{t,\delta} = u'l/\nu_\delta$, Δx is the grid spacing, and T_{peak}^F and T_{peak}^T are the location in T -space of peak fuel consumption rate and HRR in a laminar flame, respectively. In all cases, $L = 5.26l$. The other parameters are defined in the text. The laminar flame quantities are obtained with FlameMaster [25].

To independently study the effect of pressure, the Karlovitz number at the reaction zone $Ka_\delta = \delta^2/\eta_\delta^2$ [15], with δ the reaction zone thickness (evaluated as in Ref. [15]) and η_δ the Kolmogorov length scale evaluated at

the reaction zone, is fixed in a set of three simulations (P1T3, P20T3, and P20T8), for which pressure P_0 and the unburnt temperature T_u are varied. The Karlovitz number at the reaction zone was shown to be more relevant than the Karlovitz number computed in the unburnt gas Ka_u to characterize the structure of the reaction zone [15], where $Ka_u = t_F/t_{\eta_u}$, with the flame time $t_F = l_F/S_L$ and the Kolmogorov characteristic time evaluated as $t_{\eta_u} = (\nu_u l/u'^3)^{1/2}$, l_F is the laminar flame thickness, S_L the laminar flame speed, u' the rms of the velocity fluctuations, and ν_u the kinematic viscosity in the unburnt gas. In particular, effects of turbulence relaminarization are accounted for by considering Ka_δ instead of Ka_u [15]. For the present simulations, Ka_δ was chosen to be representative of the flames identified in Ref. [8]. Note that Ka_u varies from 16 to 234 between these simulations. This is due to the shift of the reaction zone towards higher temperature with increased pressure in addition to the effect of increased unburnt temperature [15].

The l/l_F ratio is fixed throughout the simulations. To limit the computational cost, a ratio of unity is chosen, which was also used in Ref. [13, 15], and is of the same order as that found in the slot burner flames of Sankaran *et al.* [33]. With both Ka_δ and l/l_F fixed, the turbulent Reynolds number at the reaction zone cannot be kept exactly constant between the three simulations.

A fourth simulation is chosen to match Ka_u of simulation P20T3, but with a pressure of 1 bar. This allows a direct comparison of the effect of pressure at constant Ka_u .

Each simulation cost approximately 150k core-hours on NERSC's cluster Hopper (performed in parallel on 1920 cores).

3. Results

3.1. Overview and global quantities

Contours of HRR are presented in Fig. 2 on which are superimposed the isocontours of temperature for T_{peak}^F and T_{peak}^T (see Table 1). As expected, the reaction zone is thin in all cases. Relatively large chemical source term fluctuations can be identified in all flames. Such fluctuations were previously found to correlate with curvature [14], which scales like the Kolmogorov length scale at the reaction zone. Larger scales (up to L) can also be identified in Fig. 2. We attribute these scales to turbulence and not to Darrieus-Landau instabilities given the current regime of combustion [34].

Figure 3 presents the conditional means of the HRR in temperature space. These are compared to the profiles in the corresponding laminar flames. While the laminar profiles differ considerably from one another, the effect of turbulence on the conditional means is comparable between the four cases. The peak values from these conditional

Fig. 2: Contours of HRR normalized by its peak laminar values, with values ranging from 0 to 1.1. The isotherms corresponding to the peak fuel consumption rate (green solid line) and the peak HRR (blue solid line) in laminar flames are also shown. Unburnt to burnt is from left to right. The heights of the slices are the respective domain widths (L), *i.e.* 2.1, 2.1, 0.24, and 0.11 mm from left to right.

Fig. 3: Conditional mean of HRR vs. temperature, normalized by the peak laminar values. The laminar profiles are shown with dashed lines.

means are listed in Table 2. The location of these peaks in T -space will be denoted T_{peak} for future reference. At constant Ka_δ (Cases P1T3, P20T3, and P20T8), there is no significant effect of pressure on the mean HRR. The effect of pressure is also very limited at constant Ka_u (Cases P1T3' and P20T3).

The mean HRR is a quantity of relevance to tabulated chemistry [35] or conditional moment closure [36] modeling approaches, but its value at T_{peak} can also be seen as an approximation for the stretch factor used with flame surface density closure models [37], *i.e.* it approximates the mean normalized consumption speed along the reaction surface [14]. A better approximation that accounts for fluctuations in reaction zone thickness can be computed as

$$I_0 = \frac{\langle \dot{\omega}_T / |\nabla T| | T_{\text{peak}} \rangle}{(\dot{\omega}_T / |\nabla T|)_{\text{peak,lam}}}. \quad (8)$$

The values for I_0 are listed in Table 3 along with the normalized turbulent flame reaction surface ($T = T_{\text{peak}}$) area. The approximate stretch factor is nearly constant between all cases, independent of pressure. However, non-negligible differences in turbulent surface areas can be identified. The product of the approximate stretch factor

Case	$\dot{\omega}_T/\dot{\omega}_{T,\text{lam}}$ at T_{peak}^T	
	Mean	Std
P1T3	0.76	0.29
P1T3'	0.77	0.26
P20T3	0.79	0.20
P20T8	0.79	0.20

Table 2: Conditional mean and standard deviation of the HRR on the isosurfaces corresponding to their respective temperature of peak mean source term (peaks in Fig. 3).

Case	$\frac{A_T}{A}$	I_0	$\frac{A_T}{A} I_0$	$\frac{S_T}{S_L}$
P1T3	1.94	0.85	1.65	1.80
P1T3'	2.24	0.89	1.99	2.05
P20T3	2.31	0.88	2.03	2.25
P20T8	1.89	0.90	1.70	1.75

Table 3: Normalized turbulent surface area A_T/A , stretch factor I_0 , and normalized turbulent flame speed S_T/S_L .

with the normalized turbulent surface area shows relatively good agreement with the normalized turbulent flame speeds (computed from the integrated fuel consumption rate as in Ref. [14]). This result indicates that differences in turbulent flame speed between the cases are caused by differences in turbulent surface area, rather than differences in stretch factor. This is consistent with the effect of pressure observed in the corrugated and wrinkled flamelet regimes [2, 5–7]. No other significant effect of pressure was identified in this section.

Note that the present small domain width constrains the flame shape modes but the effect of turbulence on the chemical source terms and on small scale wrinkling of the reaction zone was found to be independent of the domain width in similar flames [16].

3.2. Global chemical pathways

Chemical pathways in laminar flames are known to be significantly affected by pressure. In order to assess if turbulence affects these pathways in different ways, the reactions with the largest fractional contributions to the integrated fuel HRR in laminar flames are identified first. Between the three laminar flames, four common most contributing reactions were identified (Table 4). Their fractional contributions in the laminar flames are shown in Fig. 4 (left most bars for each set of color). Unsurprisingly, the fractional contributions are different between the three flames. The differences are particularly important between the high and low pressure flames.

The fractional contributions in the turbulent flames are also presented in Fig. 4. Similar to the results of Ref. [15] turbulence has virtually no global effect on the most contributing chemical reactions. This result is independent of pressure.

#	Reaction
13	$\text{H} + \text{O}_2 + \text{M4} \rightleftharpoons \text{HO}_2 + \text{M4}$
20	$\text{HO}_2 + \text{OH} \rightleftharpoons \text{H}_2\text{O} + \text{O}_2$
31	$\text{CO} + \text{OH} \rightleftharpoons \text{CO}_2 + \text{H}$
G52	$\text{CH}_3 + \text{O} \rightleftharpoons \text{CH}_2\text{O} + \text{H}$

Table 4: Chemical reactions with the largest fractional contribution to the integrated HRR in laminar flames.

Fig. 4: Fractional contribution of the reactions listed in Table 4 to the integrated HRR in both laminar and turbulent flames.

3.3. Local heat release rate distribution

Fig. 5(a) presents the distribution of HRR (with the mean and standard deviation listed in Table 2), Fig. 5(b) its mean dependence on curvature, and Fig. 5(c) the distribution of curvature on the isosurface corresponding to $T = T_{\text{peak}}$. The distributions are surface weighted (spatial average) and averaged in time. Curvature is defined as $\kappa = \nabla \cdot \mathbf{n}$, where the normal to the reaction zone $\mathbf{n} = -\nabla T/|\nabla T|$ is positive towards the unburnt gas. Effects of pressure at constant Ka_δ and Ka_u on the HRR distribution can be identified from these figures. They are each discussed below.

Fig. 5: Distribution of HRR (a), conditional mean of HRR vs. curvature (b) and distribution of curvature (c) on the isosurface corresponding to $T = T_{\text{peak}}$.

First, at constant Ka_δ , the low pressure flame exhibits a much wider HRR distribution (Fig. 5(a)). This is due to its significantly larger sensitivity to curvature (Fig. 5(b)), given that the curvature distributions are comparable between the three flames (Fig. 5(c)). These differences in sensitivity can be explained by a combination of differential diffusion and chemistry effects. In regions of high curvature, differential diffusion causes variations in local composition. The reactions that contribute to HRR involve many different species and are therefore more or less affected by these variations in local composition. Since the fractional contributions to HRR from these reactions differ between the low and high pressure cases (Fig. 4), the cumulative effect is a difference in HRR sensitivity to curvature. Note that the decrease in mean HRR with increasing curvature (in absolute value) is consistent with the sign of the Markstein numbers in laminar flames for the present mixtures [38].

Second, at constant Ka_u , the mean dependences of HRR on curvature are similar. Therefore, the increase in HRR variance for case P1T3' (Fig. 5(a)) can be attributed to the increase in curvature variance (Fig. 5(c)). This increase in variance is not surprising since the largest values of curvature present at the reaction zone are expected to scale like the inverse of the Kolmogorov length scale at that same location.

The fact that the mean dependence of HRR on curvature weakens from case P1T3 to P1T3', which have the same chemical pathways (Fig. 5(c)), can be attributed to an attenuation of differential diffusion effects through an increase in turbulent diffusivity [39, 40]. This effect was found to be highly dependent on Ka_δ [15].

4. Conclusions

The effect of pressure on heat release rate of *iso*-octane/air turbulent premixed flames in the thin reaction zones regime has been isolated from effects of Karlovitz number, Lewis numbers, and ratio of integral length scale to laminar flame thickness in a series of direct numerical simulations.

Three main conclusions were identified. First, the mean heat release rate (or the stretch factor) was found to be independent of pressure, such that the turbulent flame speed was proportional to the turbulent reaction zone surface area. Second, while the main chemical pathways in laminar flames differ considerably between the low and high pressure flames, these remained globally unaffected by turbulence in all the flames considered, independent of pressure. Finally, local heat release rate distribution was found to be affected by pressure. At constant unburnt Karlovitz number, pressure reduces the second moment of the distribution through a decrease in local curvature variance. At constant Karlovitz number at the reaction zone, pressure reduces the variance of heat release rate by affecting its mean dependence to curvature through differential diffusion-chemistry effects.

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