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Proceedings of the Combustion Institute 000 (2016) 1–7
Proceedings of the Combustion Institute
www.elsevier.com/locate/proci

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

Bruno Savard [a,*], Simon Lapointe [b], Andrzej Teodorczyk [a]

[a] *Institute of Heat Engineering, Warsaw University of Technology, Warsaw 03-729, Poland*
[b] *Graduate Aerospace Laboratories, California Institute of Technology, Pasadena, CA 91125, USA*

Received 4 December 2015; accepted 13 July 2016
Available online xxx

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 Caltech-Mech). 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

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

* Corresponding author.
E-mail addresses: bruno.savard@gmail.com, bsavard@caltech.edu (B. Savard).

http://dx.doi.org/10.1016/j.proci.2016.07.056
1540-7489 © 2016 by The Combustion Institute. Published by Elsevier Inc.

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 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

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

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

$$\frac{\partial}{\partial t}(\rho Y_i) + \nabla \cdot (\rho \boldsymbol{u} Y_i) = -\nabla \cdot \boldsymbol{j_i} + \dot{\omega}_i, \tag{3}$$

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

where ρ is the mixture density, $\boldsymbol{u}$ is the velocity, p is the hydrodynamic pressure, $\boldsymbol{\sigma}$ is the viscous stress tensor, $\boldsymbol{f}$ 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, $\boldsymbol{j_i}$, is expressed as

$$\boldsymbol{j_i} = -\rho D_i \frac{Y_i}{X_i} \nabla X_i - \rho Y_i \boldsymbol{u_c}, \tag{5}$$

where X_i is the species mole fraction and D_i is the species diffusivity. The correction velocity $\boldsymbol{u_c}$ is present to ensure zero net diffusion mass flux [20].

Please cite this article as: B. Savard et al., Numerical investigation of the effect of pressure on heat release rate in *iso*-octane premixed turbulent flames under conditions relevant to SI engines, Proceedings of the Combustion Institute (2016), http://dx.doi.org/10.1016/j.proci.2016.07.056