



# Low-temperature chemistry in *n*-heptane/air premixed turbulent flames



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## ABSTRACT

The effects of low-temperature chemistry (LTC) on *n*-heptane/air premixed turbulent flames in the thin reaction zones regime are investigated using direct numerical simulations (DNS) with reduced multi-step chemistry (129-species, 1234-reaction mechanism reduced from CaltechMech). An initial mixture of *n*-heptane/air at an equivalence ratio of 0.7, unburnt temperature of 650 K, and atmospheric pressure, which is in the negative temperature coefficient (NTC) region, is considered. The focus is put on three separate aspects: 1) LTC in turbulent hot flames propagating in this unburnt (fresh) mixture, 2) turbulent hot flames (with LTC) propagating in a mixture that has undergone first-stage ignition, and 3) turbulent cool flames. These types of flames can all be encountered in modern gasoline compression ignition and diesel engines for example. For the first aspect, it is found that LTC has negligible effect for the conditions considered. For the second aspect, at constant Karlovitz number, the increase in turbulent flame speed (relative to that of turbulent hot flames propagating in the unburnt mixture) due to partial ignition of the reactants is attributed to the increase in laminar flame speed, as opposed to turbulence–LTC interaction. Furthermore, the reaction zone is affected by turbulence in the same way as hot flames propagating in an unburnt mixture. For the third aspect, the first DNS of turbulent cool premixed *n*-heptane/air flames are presented. Under the current conditions, the initial laminar cool flames are strongly affected by auto-ignition, which is expected to occur under engine conditions, and has an ignition front structure. As the turbulent flames develop, turbulent diffusion becomes sufficiently large to initiate self-propagation of the cool flames. The flames are observed to propagate upstream steadily until they reach the inlet. The steady-state turbulent flames are found to have a highly distributed reaction zone. Nevertheless, their reaction zone structure is found to approach that of the reference (self-propagating) laminar flame (which is significantly different than that of the initial ignition fronts). In addition, this strong turbulence does not affect the global chemical pathways compared to those in the reference laminar flame. Finally, their normalized turbulent flame speed is comparable to that of hot flames at similar Karlovitz numbers.

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## 1. Introduction

Turbulent premixed flames play a major role in modern combustion devices, such as internal combustion engines and gas turbine combustors. These premixed flames often involve large hydrocarbon fuels and typically fall in the thin reaction zones (TRZ) regime [1–4]. A particularity of these fuels is their low-temperature chemistry (LTC) behavior including a two-stage

ignition in the negative temperature coefficient (NTC) region [5,6]. Under such conditions, flames that involve only LTC, cool flames, are in general associated with low heat release rate and, hence, a small increase in temperature across the flame. However, their products have increased reactivity (in terms of high-temperature chemistry) compared to that of the reactants and therefore affect hot flames propagating in their products. In gasoline engines, LTC is suspected to largely affect the occurrence of knock [7], while in low-temperature combustion diesel engines (locally partially premixed), it is argued to strongly affect the stabilization of spray flames [8]. Understanding premixed turbulent flames involving LTC in turbulence conditions associated with the TRZ regime can therefore lead to a significant impact on engine design. Note that while

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## Nomenclature

|                       |  |
|-----------------------|--|
| $\alpha$              | mixture thermal diffusivity (dimensions: $L^2T^{-1}$ )   |
| $\rho$                | density (dimensions: $ML^{-3}$ )   |
| $P$                   | pressure (dimensions: $ML^{-1}T^{-2}$ )  |
| $P_0$                 | thermodynamic pressure (dimensions: $ML^{-1}T^{-2}$ )  |
| $p$                   | hydrodynamic pressure (dimensions: $ML^{-1}T^{-2}$ )   |
| $t$                   | time (dimension: T)  |
| $\mathbf{x}$          | physical coordinate (dimension: L)   |
| $\mathbf{u}$          | velocity (dimensions: $LT^{-1}$ )  |
| $\mathbf{f}$          | turbulence forcing term (dimensions: $ML^{-2}T^{-2}$ )   |
| $\boldsymbol{\sigma}$ | viscous stress tensor (dimensions: $ML^{-1}T^{-2}$ )   |
| $\mathbf{j}_i$        | $i$ th species diffusion mass flux (dimensions: $ML^{-2}T^{-1}$ )                                    |
| $\mathbf{u}_c$        | correction velocity (dimensions: $LT^{-1}$ )   |
| $T$                   | temperature (dimension: $\Theta$ )   |
| $Y_i$                 | $i$ th species mass fraction (dimensionless)   |
| $X_i$                 | $i$ th species mole fraction (dimensionless)   |
| $c_{p,i}$             | $i$ th species heat capacity (dimensions: $L^2T^{-2}\Theta^{-1}$ )                                   |
| $c_p$                 | mixture heat capacity (dimensions: $L^2T^{-2}\Theta^{-1}$ )  |
| $\dot{\omega}_i$      | $i$ th species production rate (dimensions: $ML^{-3}T^{-1}$ )  |
| $\dot{\omega}_T$      | temperature production rate (dimensions: $ML^{-3}T^{-1}\Theta$ )                                     |
| $D_{i,m}$             | $i$ th species mixture-averaged diffusivity (dimensions: $L^2T^{-1}$ )                               |
| $\mathcal{D}_{ij}$    | binary diffusion coefficient of $i$ th species relative to $j$ th species (dimensions: $L^2T^{-1}$ ) |
| $W$                   | mixture molar weight (dimension: M)  |
| $R$                   | universal gas constant (dimensions: $ML^2T^{-2}\Theta^{-1}$ )  |
| $S_L$                 | laminar flame speed (dimensions: $LT^{-1}$ )   |
| $l_F$                 | laminar flame thickness (dimension: L)   |
| $l$                   | integral length scale (dimension: L)   |
| $u_{in}$              | inflow velocity (dimensions: $LT^{-1}$ )   |
| $u'$                  | root-mean-square of velocity fluctuations (dimensions: $LT^{-1}$ )                                   |
| $L_f$                 | flame stabilization position (dimension: L)  |
| $Ka_u$                | Karlovitz number in the unburnt mixture (dimensionless)  |
| $Ka_\delta$           | Karlovitz number at the reaction zone (dimensionless)  |
| $t_F$                 | flame time (dimension: T)  |
| $t_{\eta u}$          | Kolmogorov time scale in the unburnt mixture (dimension: T)  |
| $\nu_u$               | kinematic viscosity in the unburnt mixture (dimensions: $L^2T^{-1}$ )                                |
| $\delta$              | reaction zone thickness (dimension: L)   |
| $L$                   | cross-section height of the computational domain (dimension: L)                                      |
| $S_T$                 | turbulent flame speed (dimensions: $LT^{-1}$ )   |
| $A_T$                 | turbulent surface area (dimensions: $L^2$ )  |
| $A$                   | cross-section area of the computational domain (dimensions: $L^2$ )                                  |
| $Re_{t,u}$            | turbulent Reynolds number in the unburnt mixture (dimensionless)                                     |
| $x_f$                 | instantaneous flame position (dimension: L)  |
| $c_b$                 | progress variable in the burnt mixture (dimensionless)   |
| $c$                   | progress variable (dimensionless)  |
| $\Omega$              | volume contained by the computational domain (dimensions: $L^3$ )                                    |
| $\tau$                | integral eddy turnover time (dimension: T)   |
| $l_0$                 | burning efficiency factor (dimensionless)  |
| $\delta_T$            | turbulent reaction zone thickness (dimension: L)   |

|      |  |
|------|--|
| DNS  | direct numerical simulation                |
| LTC  | low-temperature chemistry                  |
| HTC  | high-temperature chemistry                 |
| HRR  | heat release rate                          |
| UM   | unburnt mixture                            |
| PDF  | probability density function               |
| PIM  | partially ignited mixture                  |
| CF   | cool flame                                 |
| TKE  | turbulent kinetic energy                   |
| TRZ  | thin reaction zones                        |
| HCCI | homogeneous charge compression ignition    |
| RCCI | reactivity controlled compression ignition |
| NTC  | negative temperature coefficient           |

partial or imperfect premixing is often encountered in engines, we limit the scope of the present study to premixed flames in an effort to simplify and target the analysis. In addition, we recall that other combustion regimes beyond the scope of this study, such as the corrugated flamelet regime, are also relevant to engine combustion.

The impact of LTC on turbulence–chemistry interaction in the TRZ regime is investigated in the present work by considering the following three situations:

1. hot flames propagating in an unburnt (fresh) mixture of reactants under conditions corresponding to the NTC region,
2. hot flames propagating in a mixture that has undergone first stage ignition (in the NTC region), and
3. cool flames.

While case (i) is relevant to any flame in the TRZ regime with fuels characterized by LTC, cases (ii) and (iii) relate to situations in which the reactants are subject to sufficient residence time to experience LTC before encountering the hot flame [9], such as in low-temperature combustion diesel engines [8], practical homogeneous charge compression ignition (HCCI) [10,11] and fuel reactivity controlled compression ignition (RCCI) [12] engines, and can occur in gasoline engines [7]. In fact, all three types of flames can be encountered in these engines and they can possibly interact with each other.

Premixed turbulent flames in the TRZ regime have been studied theoretically (e.g. [13–17]), experimentally (e.g. [18–22]) and numerically (e.g. [23–32]) in the past few years. In this regime, thickened preheat zones with thin reaction zones have been clearly observed (e.g. [19,25]). While the reaction zone remains thin, it was shown to be strongly affected by turbulence, especially with large hydrocarbon fuels [25–27,31]. The dependence of this turbulence–chemistry interaction on Lewis number [26–28], unburnt temperature [27,29], background pressure [29], and chemical kinetic mechanism [33] have been previously investigated using direct numerical simulations (DNS). However, none of these studies have investigated the effect of LTC. Experimental work in this regime remains limited due to its challenging complexity and, to the best of the authors' knowledge, the effect of LTC on premixed flames in the TRZ regime propagating in an unburnt mixture of reactants has not been investigated yet. While Carbone et al. [21] have recently conducted experiments on premixed turbulent jet flames in the TRZ and broken reaction zones regimes with up to  $C_7$  linear alkane fuels, the thermodynamic conditions considered remained far outside the NTC region.

Recently, the effect of partial ignition (low-temperature, first-stage ignition) on turbulent flame speed has been investigated experimentally with the Princeton RATS burner [9,34]. In a first paper, Won et al. [9] observed a significant increase in turbulent flame speed, at constant turbulence intensity, as the reactant

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