

Numerical investigation of large scale effects on turbulent premixed flames

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Abstract

Large scale effects on premixed flames are numerically investigated in both laminar and moderately turbulent flow fields using two-dimensional direct numerical simulations. A low-Mach number formulation of the governing equations is used in conjunction with a deficient reactant formulation enabling a coherent use of results obtained within the context of asymptotic hydrodynamic theory of premixed flames. This feature is of particular importance to study Darrieus-Landau (DL) or hydrodynamic instability which is characterized by a long wavelength nature. Therefore it is particularly important in *large scale* flames and large scale combustion devices where it is expected to be ubiquitous. A dual behavior stable/unstable is observed, in both laminar and moderately turbulent flames, varying the reference hydrodynamic length moving from small to large scale flames.

1. Introduction

The study of turbulent premixed combustion is of great importance for many practical applications and it poses a wide range of theoretical, numerical and experimental challenges due to its multi-scale and highly non-linear nature. Interactions between a reactive flame front and a turbulent flow field still require a substantially deeper understanding in order to improve the limited predictive capabilities of the currently available combustion models [1, 2]. In this context direct numerical simulation (DNS) is a fundamental tool for the study turbulent premixed combustion without modeling combustion and/or turbulent motion [3]. However the extremely high computational costs of performing DNS limits the condition range that can be explored by the simulations [4]. Despite these limitations recently many research groups have been capable of investigating relevant turbulent premixed flame using 3D DNS and relatively chemical mechanisms [5, 6, 7]. The synergies between experimental and numerical researchers is now driving to *DNS-oriented* experiments, thus experimental configurations that can be simulated by means of currently available DNS codes and computational resources. Following this approach many relevant results have been obtained [8] and many others can be expected in the near future. Nevertheless, DNS studies using substantially simplified assumptions on chemistry, heat release as well as dimensionality (2D instead of 3D) remain of great importance and interest from a basic point of view [9].

In the present work we numerically investigate large scale effects on turbulent premixed flames in a moderately turbulent flow field using two-dimensional DNS. This effort is envisaged as a preliminary step toward the three-dimensional simulations. The governing equations are formulated in the low-Mach number limit together with a deficient reactant formulation which enables a coherent use of the linear stability

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analysis [10]. The latter is of particularly useful studying the often overlooked effects of intrinsic Darrieus-Landau (DL) or hydrodynamic instability [11, 12].

Indeed, recent numerical efforts generally focus on the investigation of high Karlovitz number flames [14] and the resulting effect of the smallest turbulent (Kolmogorov) scales on flame propagation. This highly demanding task in terms of spatial resolution generally limits the investigation to small lateral domains and as a consequence, the ratio of lateral domain size to flame thickness $\hat{\delta}$ is rarely above 10. For such *small scale* flames, hydrodynamic instability effects are almost invariably suppressed as the lateral flame size is smaller than the smallest (cut-off) unstable perturbation wavelength. On the contrary, the long wavelength nature of DL instability makes it particularly important in *large scale* flames and large scale combustion devices where it is expected to be ubiquitous. In this context, the term large scale may be related to flames for which the ratio of lateral domain size to flame thickness is of the order of $\hat{\delta} \sim 100$. Table 1 summarize some of the recent DNS of turbulent premixed combustion evidencing their relative $\hat{\delta}$.

Table 1: Recent DNS studies

Hydrodynamic length	Flame thickness	$\hat{\delta}$	Points	Code	Reference
1.50mm	0.66mm	2.27	2.0Bil	S3D	[8]
4.33mm	0.44mm	9.84	2.7Bil	CIAO	[7]
2.59mm	0.32mm	0.89	4.3Bil	AthenaRX	[13]
2.33mm	0.39mm	5.97	0.2Bil	NGA	[14]

Turbulent premixed combustion can be largely influenced by the onset of Darrieus-Landau (DL) or hydrodynamic instabilities [15, 16], especially in mildly turbulent conditions. Such effects are to be considered independent and of different nature with respect to high Karlovitz effects. In a recent work [17] the features of DL-affected premixed turbulent flames were investigated both numerically and experimentally, highlighting the bifurcative role of domain size on both flame morphology and propagation speed. In the present work we draw from the results of [17] and delve deeper in the features of stable/unstable turbulent flames in terms of large scale effects proposing an alternative non-dimensionalization of the governing equations.

2. Theoretical and numerical formulation

To study large scale premixed flames subject to DL instability, we adopt a one-step irreversible Arrhenius reaction model in which the reaction rate is determined by a deficient reactant. The latter is completely depleted across the flame while the concentration of other reactants remains essentially unchanged, hence the reacting mixture is sufficiently off-stoichiometric. Therefore all the transport properties can be considered constant since they are not influenced by the presence/absence of the deficient reactant. The use of the deficient reactant model enables the coherent use of results obtained within the asymptotic hydrodynamic theory of premixed flames developed in [10] and in particular the linear stability properties of flames derived therein.

Operatively we nondimensionalize spatial variables with respect to a critical hydrodynamic wavelength λ_c , which can be estimated from linear stability analysis as illustrated in [17], while time is nondimensionalized by λ_c/S_L^0 . Other nondimensional variables, such as density and mass fraction of the deficient reactant, are measured in units of ρ_u , where the subscript u denotes the value in the unburned fresh mixture, while velocities are measured in units of S_L^0 . The nondimensional temperature is defined as $\theta = T - T_u / (T_{ad} - T_u)$, where T is the dimensional temperature and T_{ad} is the adiabatic flame temperature, i.e., the temperature

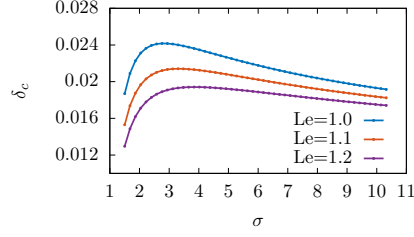


Figure 1: Dimensionless flame thickness δ_c as function of the expansion ratio σ for three Lewis numbers.

downstream of an adiabatic unstretched planar flame. The ensuing non-dimensional form of the governing equations reads:

$$\rho \frac{D\mathbf{u}}{Dt} = -\nabla p_2 + \delta_c Pr \nabla \cdot (\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - \frac{2}{3} (\nabla \cdot \mathbf{u}) \mathbf{I} \quad (1)$$

$$\rho \frac{D\theta}{Dt} = \nabla \cdot (\delta_c \nabla \theta) + \frac{\dot{\omega}}{\delta_c} \quad (2)$$

$$\rho \frac{DY}{Dt} = \nabla \cdot \left(\frac{\delta_c}{Le} \nabla Y \right) - \frac{\dot{\omega}}{\delta_c} \quad (3)$$

while the continuity equation is replaced by a constrain on the velocity divergence:

$$\nabla \cdot \mathbf{u} = (\sigma - 1) \left[\nabla \cdot (\delta_c \nabla \theta) + \frac{\dot{\omega}}{\delta_c} \right] \quad (4)$$

where the non-dimensional state variables are the velocity $\mathbf{u}$, is the deficient reactant mass fraction Y and the non dimensional temperature $\theta = T - T_u / (T_{ad} - T_u)$ being T_u the unburned mixture temperature and T_{ad} . The source/sink term and the equation of state are expressed as:

$$\dot{\omega} = \frac{Ze^2}{2Le} Y \exp\left(\frac{Ze(1-\theta)}{1 - (1 - \frac{1}{\sigma})(1-\theta)}\right) \quad \rho = \frac{1}{(\sigma - 1)\theta + 1} \quad (5)$$

The non-dimensional parameters are defined as:

- expansion ratio $\sigma = \frac{\rho_u}{\rho_b}$ where subscript u and b are referring to the unburned and burnt regions.
- dimensionless flame thickness $\delta_c = \frac{l_d}{\lambda_c}$ where $l_d = \lambda / \rho_u c_p S_L^0$ is the dimensional flame thickness and λ_c the dimensional critical hydrodynamic wave length, that can be estimated following [17].
- Lewis number $Le = \frac{k}{\rho_u c_p D}$ where k is the thermal conductivity, c_p the constant pressure specific heat and D the diffusivity of the deficient reactant.
- Zeldovich number $Ze = \frac{T_a(T_{ad} - T_u)}{T_{ad}^2}$ where T_{ad} is the adiabatic flame temperature.
- Prandtl number $Pr = \frac{\nu}{k}$ where ν is kinematic viscosity.

It is important to remark that in this form of the non dimensional equations, contrary to [17], all the parameters are function of the mixture only. A modified version of the highly parallel, spectral element, incompressible and low-Mach number code nek5000 [18] is used to solve numerically the discretized system.

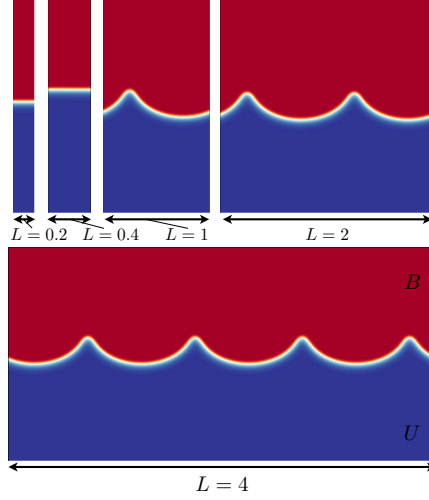


Figure 2: Two-dimensional laminar flames downward propagating for various domain width L .

3. Results and Discussion

In order to investigate large scale premixed flames possibly subject to DL instability a set of mixture dependent parameters, are chosen in order to be representative of lean/rich hydrocarbon combustion: $\sigma = 3$, $\delta_c = 0.02414$, $Le = 1.0$, $Ze = 6.0$ and $Pr = 0.1$. Moreover these parameters have been also chosen to obtain an elevated δ_c as shown in Fig. 1, which governs the grid resolution requirements for two-dimensional DNS.

Once the mixture parameters are fixed, the only other parameter to be set, in a laminar scenario is the hydrodynamic length $\hat{L}$. For planar flames the reference hydrodynamic length is simply the domain width. The maximum number of unstable wavelengths (or unstable cells) n_c contained in the domain can be defined as $n_c = \hat{L}/\lambda_c$, which corresponds to the nondimensional domain width L . Therefore for a domain characterized by $L < 1$ the planar flame is expected to be stable (i.e. possessing a fractional number of unstable cells), while for $L > 1$ the planar flame front is expected to be unstable and thus exhibit an integer number of unstable cells. In this latter case the flame morphology is expected to be corrugated by DL instability.

Figure 2 shows laminar flames propagating downward for various domain width L . It is clearly observable the dual behavior of the flame depending on the hydrodynamic length. The planar flames with $L > 1$ are corrugated by DL instability, exhibiting the characteristic cusp-like structures. Note that the number of unstable cells present in such domains is comprised between 1 and n_c depending on the initial small perturbation imposed.

Figure 3 shows the same dual behavior also in a moderately turbulent scenario, using different domain width: small $L = 0.5$, medium $L = 2.0$ and large $L = 10.0$. For these turbulent cases, homogeneous isotropic turbulence is superimposed to the incoming flow characterized by a perturbation intensity $u' = 1.0$ and an integral length scale $l_0 = 0.1$. The three flames are located in the same position in a Borghi type diagram [3] having the same u'/S_L^0 and l_0/l_d . However the flame behavior is completely different since the $L = 2.0$ and $L = 10.0$ case are greatly influenced by large scale DL instabilities. This can be considered an issue related to large scale flame since the ratio between the domain width and the flame thickness are $\hat{\delta} = L/\delta_c \sim 83$ and $\hat{\delta} = L/\delta_c \sim 414.2$ respectively. This suggest particular care in addressing the investigation of *large scale* flames and large scale combustion devices. The DL effects in such flames it is expected to be ubiquitous and

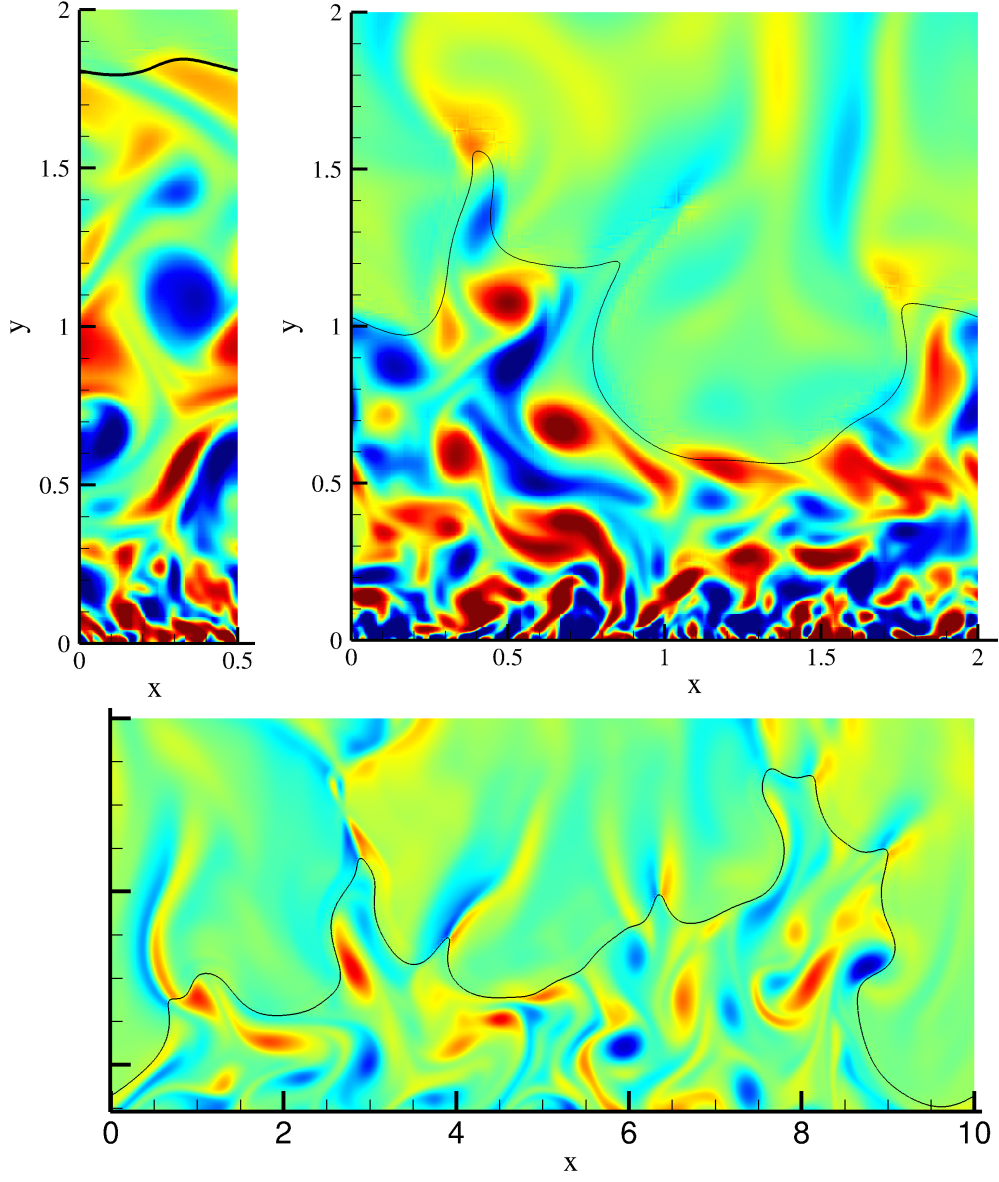


Figure 3: Instantaneous vorticity flow-field of two turbulent flames with $L = 0.5$, $L = 2.0$ and $L = 10.0$ ($\hat{\delta} = 20.7$, $\hat{\delta} = 82.8$ and $\hat{\delta} = 414.2$ respectively). The continuous black line is the $Y = 0.5$ isocontour representing the position of the flame front.

therefore to be taken into account in context of turbulent combustion modeling for LES/RANS approaches.

4. Conclusion and perspective

Large scale effects on premixed combustion have been numerically investigated using two-dimensional DNS of planar premixed flames. A dual behavior stable/unstable has been observed, in both laminar and moderately turbulent flames, varying the reference hydrodynamic length moving towards large scale flames. With the presented non-dimensionalization, consistently with asymptotic hydrodynamic theory, DL driven corrugations have been observed in flames propagating in domains larger than $L = 1$. These turbulent flames have been shown to be greatly influenced by large scale DL instabilities suggesting particular care in the investigation of large scale combustion devices.

Acknowledgements

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