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Direct numerical simulation of circular expanding premixed flames in a lean quiescent hydrogen-air mixture: Phenomenology and detailed flame front analysis

Christos Altantzis [a,1], Christos E. Frouzakis [a,*], Ananias G. Tomboulides [b], Konstantinos Boulouchos [a]

[a] Aerothermochemistry and Combustion Systems Laboratory, Swiss Federal Institute of Technology, Zurich CH-8092, Switzerland
[b] Department of Mechanical Engineering, University of Western Macedonia, 50100 Kozani, Greece

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ABSTRACT

The transition to cellularity and the dynamics of lean premixed hydrogen/air flames propagating outwards in 2D circular domains under the combined influence of the hydrodynamic and thermodiffusive instabilities is investigated computationally using detailed chemistry and transport. In response to monochromatic (single wavelength) and polychromatic perturbations imposed initially on the flame, the non-monotonic rate of increase of the surface area reflects the transitions of the perturbed front dynamics. The relation of the wavelength of the cellular structures with the growth rate of their amplitude is investigated separately during the initial interval of accelerated growth marking the onset of cellularity as well as during later times when the wrinkled front undergoes a continuous process of cell creation and annihilation. As the flame expands, the local minima of the initial perturbation determine the primary troughs which have a dominant effect on the long term evolution since they constrain the waveangle over which secondary cells can form and interact and define the periodicity of the problem. During the time interval of propagation considered in this study, it is found that the temporal evolution of the mean flame radius does not follow a power law, but varies almost linearly in time.

1. Introduction

The propagation characteristics and the prediction of the integral heat release rate following the ignition of a combustible premixed mixture are of interest in many combustion applications. In the absence of turbulence, premixed flame fronts become wrinkled by different mechanisms [1]: the hydrodynamic instability [2,3] caused by the omnipresent density jump across the flame, the thermal-diffusive instability [4] stemming from the diffusion imbalance between heat and mass of the deficient reactant, and the buoyancy-driven Rayleigh–Taylor instability [1].

The 2-D circular flame lies between the planar flame which has been investigated extensively theoretically (e.g., [1,5–7]) as well as numerically (e.g., [8–10]), and the experimentally convenient spherical flame (see, for example, [11–13]). Recent investigations of outwards propagating flames [13,14] showed that lean hydrogen flames at elevated pressures transition to observable cellularity significantly faster after ignition than equidiffusive mixtures. Experimental investigations of purely hydrodynamically unstable flames (e.g., [15,16,13,14]) showed that there exists a critical radius marking the transition, and furthermore that the self-acceleration due to the wrinkling of the flame front is associated with self-similar structures forming during propagation.

The temporal dependence of the mean radius of the propagating flame was found to be $R_{mean} \propto A t^{\alpha}$, with A and α being empirical constants. The experimental results were compared with results from theoretical investigations of self-acceleration (e.g., [17–19]) and 2D numerical simulations either of the model equations of Sivashinsky and Frankel (e.g., [19–22]), or by using the G-equation to model the flame front as a surface of discontinuity (e.g., [22,23]). Although self-acceleration and fractalization of the flame front was reported in all these studies, the extracted exponents did not agree. One of the very few numerical works that employed the direct solution of the reactive Navier–Stokes equations with single-step chemistry and constant transport properties, confirmed the theoretical predictions for hydrodynamically unstable 2-D expanding

* Corresponding author. Address: Aerothermochemistry and Combustion Systems Laboratory, Swiss Federal Institute of Technology (ETH), Sonnegstrasse 3, Zurich CH-8092, Switzerland. Fax: +41 44 632 1255.[1]Current address: Department of Mechanical Engineering, Massachusetts Institute of Technology, 77 Massachusetts Avenue, Cambridge MA 02139, USA.

E-mail address: frouzakis@lav.mavt.ethz.ch (C.E. Frouzakis).

[1] Current address: Department of Mechanical Engineering, Massachusetts Institute of Technology, 77 Massachusetts Avenue, Cambridge MA 02139, USA.

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flames agreeing with the value $\alpha = 1.25$ for the growth exponent [24].

The additional effect of the thermodiffusive instability mechanism results in more complicated dynamics and the behavior of the flame front is not fully understood. The theoretical analyses of [25,26] derived analytical expression for the onset of instability (critical flame radius for the appearance of cells and cell size) and the subsequent cell development on spherically expanding flames affected by hydrodynamic as well as thermodiffusive effects.

The first numerical investigation of 2-D circular flames subjected to the combined effect of both mechanisms was performed by Kadowaki [27] employing a single-step reaction between burned and unburned gases. Three Lewis numbers were considered ($Le = 0.8, 1.0, 1.2$) in order to include both the destabilizing and stabilizing effects of the diffusion imbalance. The extracted growth rates were found to be consistent with those of the planar flames when $Le = 1.0$. For Lewis number higher/lower than unity, the growth rates were found to be lower/higher than those of the planar flames. More recently, the long-time nonlinear evolution of low Lewis number 2- and 3-D cylindrical flames was investigated in [28]. Hydrogen combustion chemistry was described by a single-step reaction and the domain considered extended 100 flame thicknesses in the radial direction and, for the 3-D case, 20 flame thicknesses in the axial direction. It was found that the flame area growth and the heat release rate vary non-monotonically, a behavior which was more pronounced in the 3-D cases where the transitions in the propagating dynamics were accompanied by swapping of the troughs and crests that formed on the flame surface. During this swapping it was observed that the wrinkled flame assumed a smooth cylindrical surface before new cells could form and grow.

Detailed investigations of the coupled influence of the two instability mechanisms on laminar planar fronts was presented in [10] employing detailed chemistry for a lean ($\phi = 0.6$) H_2/air combustion at pressure 5 atm. Linear stability analysis of the planar flames provided the range of the unstable wavelengths as well as the growth rate of each wavelength, and the results were expressed by the numerically computed dispersion relation. In the following we will refer to the results reported in [10] in order to compare the amplification of perturbations imposed on the 2*D* circular fronts whose wavelength, unlike the planar front, grows in time following the expanding flame. In [29] the effects of the instability mechanisms were studied separately and compared in detail with the latest theoretical advancements using simplified chemistry.

The present work aims at investigating the onset of cellularity and the long-term propagation dynamics of 2-D thermo-diffusively unstable circular flames employing detailed descriptions of kinetics and transport. Different initial perturbations are superimposed on the flame, and the subsequent evolution of the patterns formed is studied in detail. The wrinkling of the circular front induces self-acceleration in a non-monotonic fashion, while the mean flame radius increases linearly with time. Of particular interest is the role of the local flame stretch on the propagation speed as well as on the amplification or annihilation of patterns of certain wavelengths resulting in the non-monotonic increase of the heat release rate.

2. Problem setup

2.1. Computational domain and solution method

The conservation equations for low Mach number reacting flows [30,31] presented in [29] are discretized in space using the spectral element method [32,33] in a computational domain that is split into curved-sided conforming quadrilateral elements. The solution, data and geometry are expressed as *n*th-order tensor product Legendre polynomials based on the Gauss–Lobatto–Legendre quadrature points. The discretized equations are solved with a parallel code which is based on the incompressible flow solver *nek5000* [34] using the high-order splitting scheme described in [35]. The continuity and momentum equations are integrated with a semi-implicit scheme, whereas the species and energy equations are integrated implicitly without further splitting using CVODE [36].

A lean premixed H_2/air mixture with equivalence ratio $\phi = 0.6$ is considered at temperature $\widetilde{T}_u = 298$ K and pressure $\tilde{p} = 5$ atm. Kinetics is described by the detailed mechanism of Li et al. [37], consisting of 9 species in 19 non-duplicate elementary reactions. The Chemkin transport and thermo-chemistry libraries [38,39] are used for the evaluation of the transport and thermodynamic properties and chemical reaction rates. The corresponding premixed 1-D flame structure calculated using PREMIX [40] has a thickness, defined based on the unburned flame temperature $\widetilde{T}_u$, the adiabatic flame temperature $\widetilde{T}_b = 1843.5$ K, and the maximum temperature gradient through the 1-D flame, equal to $\delta_T = (\widetilde{T}_b - \widetilde{T}_u)/\max(d\widetilde{T}/d\tilde{x}) = 7.52 \times 10^{-3}$ cm, which defines the reference length scale. The laminar flame speed $\widetilde{S}_L = 51.44$ cm/s is used as the reference velocity, resulting in a reference time (the flame transit time) $\tau = \delta_T/\widetilde{S}_L = 1.46 \cdot 10^{-4}$ s. For the conditions considered, the Lewis number of the deficient reactant is $Le_{H_2} = 0.4$ while the thermal expansion coefficient, the ratio of unburned to burned mixture density, is $\sigma = \tilde{\rho}_u/\tilde{\rho}_b = 5.56$, so that the mixture is exposed to both hydrodynamic and thermodiffusive instabilities. In the following, nondimensional variables will be used with respect to the reference values mentioned above and the temperature and properties of the unburned mixture.

Cellular flames have been found to be sensitive to background noise in a series of theoretical and numerical studies (e.g., [41–43]). Spatial discretization is a subtle issue, since the circular flame front evolution is sensitive not only to the level of the numerical noise, but also to the isotropy of the resolution. In a square domain discretized in square elements of size δ_T, the resolution is anisotropic as front segments propagating along the principal axis ($\theta = n\pi/2, n = 0, 1, 2, 3$) experience maximum resolution, while along the diagonals ($\theta = n\pi/2 + \pi/4, n = 0, 1, 2, 3$) the resolution is reduced by a factor of $\sqrt{2}$. The anisotropic resolution acts continuously as a perturbation on the propagating front, affecting its dynamics and the wavelengths of the cellular structures.

The temporal evolution of the unperturbed circular flame defined by the $T = 3$ temperature isoline expanding freely in a square domain with a side equal to $120\delta_T$ is shown in the upper right quarter of the full domain in Fig. 1(a). The flame is initialized at $R_{ig} = 11$ by interpolating the planar 1-D flame structure, and outflow boundary conditions are imposed along the domain boundaries. The thermal thickness of the planar flame is resolved by using one element per flame thickness and polynomial order $N = 18$, resulting in 18 grid points per δ_T. The initially unperturbed flame can be seen to acquire a fully cellular structure after a radius of approximately 30. Furthermore, the long-term development of the cells reflects the symmetry of the mesh, and the cellular structures along the front are symmetric with respect to the diagonals.

In order to overcome the problem with grid anisotropy, a circular domain segment was employed extending in the radial direction from an inner radius of $R_{in} = 8$ to an outer of $R_{out} = 200$, and in the azimuthal direction from $\pi/4$ to $3\pi/4$. Locally refined grids following the propagating front were employed to ensure that the flame thickness is resolved by at least the same number of points in the azimuthal and radial directions while keeping the computational cost low. Three meshes with overlapping well-resolved regions were used with 6963, 31,800 and 32,900 spectral elements and high-resolution areas extending over $8 \leqslant r \leqslant 62, 53 \leqslant r \leqslant 146$, and $137 \leqslant r \leqslant 200$, respectively. A polynomial order $N = 9$ was