

TURBULENCE-COMBUSTION INTERACTION IN H₂/CO/AIR BUNSEN FLAME

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Abstract In last decades, the increasing care to environmental safeguard and costs in the hydrocarbon fuel supplying have prompted in the development of alternative fuels, namely hydrogen based fuels as syngas. Syngas consists in a mixture of hydrogen and carbon monoxide (CO) in different relative concentration, in some cases with small concentration of methane. The aim of this work is to address the dynamics of turbulent hydrogen/carbon-monoxide/air Bunsen flames by means of Direct Numerical Simulation. The main issue is to understand how the thermo-diffusive instabilities occurring in pure hydrogen/air flame [7] are influenced by the presence of the carbon-monoxide. It is well known that the thermo-diffusive instabilities are mainly induced by the high hydrogen diffusivity leading to local quenching and temperature peaks in the flame with consequent increase of pollutant formation (e.g. NO_x). The presence of carbon monoxide in the fuel mixture has significant effects in flame dynamics where we observe a damping of the H₂/air flame instabilities with less apparent quenching and high temperature peaks.

INTRODUCTION

Alternative fuels are progressively employed to reduce the pollutant emissions and the energy production costs. Among them the most promising and studied are the hydrogen or hydrogen-based fuels. Syngas (Synthesis Gas) is a mixture of hydrogen and carbon monoxide, sometimes with small concentration of methane and carbon dioxide. It can be produced from a wide range of sources, namely the steam reforming of natural gas, gasification of coal, biomass, organic waste and refinery residuals [4]. These features make the syngas a very appealing alternative with respect to standard fossil fuels. However, its consequences on flame stability and emissions should be carefully investigated before it will be used in large-scale devices. The present work aims to fill this gap by means of Direct Numerical Simulations of H₂-CO flames in air.

METHODOLOGY

Turbulent combustion of a premixed flame of H₂-CO and air is studied by the Direct Numerical Simulation (DNS) of a turbulent Bunsen burner. The algorithm discretizes the Low-Mach number formulation of the Navier-Stokes equations in a cylindrical domain which describes a reactive flow at low Mach number with arbitrary density variations, neglecting acoustics effects. Spatial discretization is based on central second order finite differences in conservative form on a staggered grid. Low-storage third order Runge-Kutta scheme is employed for temporal integration. Turbulent velocity profile is enforced at the inflow section (Dirichlet condition) and is provided by a cross-sectional plane of a periodic turbulent pipe flow evolving simultaneously with the jet flow. A convective outflow condition is adopted together with a traction-free condition at the side boundary to mimic the open environment surrounding the flame, see [1, 9] for additional details on the code and the validation. From the chemical point of view the reduced mechanism provided in [10] with 10 species and 24 reaction is employed and the diffusivity of the involved species are considered [8]. The DNS simulations reproduce the flame in a premixed Bunsen burner with diameter-based Reynolds number $Re_D = U_0 D / \nu_\infty = 6000$, with U_0 the bulk velocity and diameter D . The parameters of the simulation correspond to a lean premixed Bunsen flame ($\phi = 0.4$, $n_{CO}/n_{H_2} = 0.5$, where n are the moles). The heat capacity ratio is $\gamma = c_p/c_v = 1.33$, while viscosity depends on temperature, $\mu \propto \sqrt{T}$. The computational domain, $[\theta_{max} \times R_{max} \times Z_{max}] = [2\pi \times 6.2D \times 7D]$, is discretized by $N_\theta \times N_r \times N_z = 128 \times 201 \times 560$ nodes with radial mesh stretching for accurate resolution of the shear layer and of the instantaneous flame front (4–5 points within the instantaneous flame thickness), see [1, 9] for details and tests. The simulation runs for more than $30 D/U_0$ to achieve the statistical steady state before collecting one hundred sample uncorrelated fields, separated by $0.125 D/U_0$, for statistical analysis.

RESULTS

The typical phenomenon occurring in a pure hydrogen air flames consists in the thermo-diffusive instability, observed both experimentally [5] and numerically [2]. As a matter of fact the high hydrogen diffusivity in presence of the flame corrugations induced by turbulence produces strong inhomogeneities in the hydrogen concentration along the flame front. This induces high heat release in the richest regions, with local overcoming of the mixture adiabatic temperature (super-adiabatic zones), and local quenching in the poorest flame regions. The suitable parameter to describe this phenomenon is

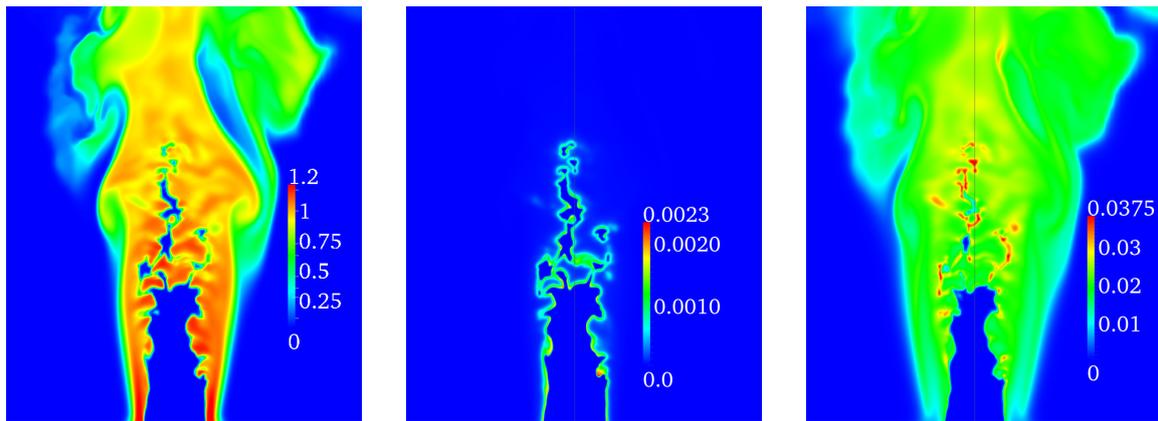


Figure 1. Instantaneous fields of Hydrogen/carbon-monoxide/air flame S2: progress variable c_T (left panel), OH concentration (middle panel) and CO_2 concentration (right panel).

the Lewis number Le , defined as the ratio between the thermal diffusivity and the mass diffusivity. When $Le < 1$ thermo-diffusive instability occurs, while a Lewis number greater than one produce a stable flame with less corrugations [3]. When flames with many species are considered, the Lewis number is usually defined with respect to the mass diffusivity of the less abundant reactant. The left panel of figure 1 shows the instantaneous temperature-based progress variable $c_T = T - T_u / (T_{ad} - T_u)$ (T temperature, T_{ad} adiabatic flame temperature, T_u unburned mixture temperature). The flame front position is easily detectable and its large corrugations are clearly apparent. The front appears severely wrinkled by turbulence even to the extent of tearing off pockets of fresh gas, which are carried into the product side where are eventually consumed. The flame front is constituted essentially by region with negative and smooth curvature (convex towards the fresh gases), and by region with positive and high curvature (convex towards the burnt gases). The negative curvature regions experience c_T values greater than unity, up to 1.2, showing the super-adiabatic behaviour that previously was referred, while in the complementary regions (positive curvature) c_T is even slightly lower than unity. Figure 1 (middle panel) shows the instantaneous concentration of the OH radicals, with its maximum value in the region with negative curvature, as observed in the pure hydrogen flame [7, 2]. On the other hand, unlike the pure hydrogen flame, no local quenching in the positive curvature region are apparent, where the OH concentration experiences non-zero value though small. The absence of the quenching regions characterizing the pure hydrogen flame is clearly explained by the CO_2 concentration instantaneous field, middle panel of figure 1. The largest production of carbon dioxide occurs in the positive curvature flame front regions where local quenching is expected. In these regions the reaction is sustained by the oxidation of the carbon monoxide and the temperature is large enough to support the OH production.

In extended work it will be shown- that the presence of carbon monoxide reduces the occurrence of quenching regions and tends to uniform the temperature fields reducing the thermo-diffusive instability particularly strong in the pure hydrogen flame. The results will be compared with a pure hydrogen flame simulation in order to better highlight the effects carbon monoxide addition on the addressed phenomenology.

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