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# Hydrogen-enriched non-premixed jet flames: Compositional structures with near-wall effects

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ABSTRACT

The species concentrations of non-premixed hydrogen and syngas flames were examined using results obtained from direct numerical simulation technique with flamelet generated manifold chemistry. Flames with pure $H_2$ and $H_2$/CO mixtures are discussed for an impinging jet flame configuration. Single-point data analyses are presented illustrating the effects of fuel composition on species concentrations. In general, scatterplots of all species show the effects of fuel variability on the flame compositional structures. The behaviours of major combustion products and key radicals species indicate the effects of CO concentration on the 2/CO syngas combustion. In particular, high concentration of CO tends to induce local extinction in the 2/CO flames in which critical chemical reactions of the fuel mixture such as CO + OH become important. The unsteady fluctuations of species profiles in the wall jet region characterise the complexity of the distributions of compositional structures in the near-wall region with respect to the effects of CO concentration on the combustion of hydrogen-enriched fuels.



## 1. Introduction

There is a great interest in the investigation on compositional structures in hydrogen-enriched syngas combustion due to their importance in the estimation of combustion products, as well as the wide range of emission issues for $H_2$-enriched combustion technologies [1–3]. Such investigation is extremely useful since compositional structures provide information on the flame structure of $H_2$-enriched syngas fuels with respect to different $H_2$ amount in the fuel compositions. In terms of the fuel compositions, syngas is mostly a mixture of $H_2$ and CO, where the unique characteristics of $H_2$ can alter the combustion process of the fuel mixture [4,5]. The analysis of compositional structures could provide a wealth of information on fluid-chemistry interaction in $H_2$-enriched reacting flows as the much-needed fundamental knowledge for clean combustion application.

One-point data analysis is a widely used technique in both experimental and computational studies of reacting flows and consists of collecting local values of relevant quantities at each point of the domain which generates scatterplots of combustion variables [6,7]. It can be used to facilitate the study of combustion mechanisms, by proving important information on both the unsteady and steady characteristics of combustion chemistry. For detailed numerical simulations of $H_2$-enriched syngas flames, the one-point data analysis of the

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computational results can be used to access the compositional structures of the flame to obtain a better understanding on the flame dynamics and would directly aid in the development of combustion models for industrial applications of clean alternative fuels as well as the design of syngas based combustion technology.

Various experimental investigations based on one-point scatter data analysis were reported in the literature. Masri et al. [6] discussed scatterplots of temperature and mass fractions of species at several locations in turbulent jet flames for flame stabilisation. Dally et al. [8] later reported compositional structures of bluff-body stabilised $H_2$/CO and $H_2$/$CH_4$ flames using scattered data analysis. Measurements of scatter data are also discussed for $H_2$/air premixed Bunsen flames [9], swirl stabilised$CH_4$, $CH_4$/Air and $CH_4$/$H_2$ non-premixed flames [10], lifted $CH_4$/air non-premixed jet flames in a vitiated co-flow [11], lifted $H_2$ jet flame [12] and partially premixed $CH_4$ flames [13]. Recently Fuest et al. [14] reported scatter data analysis of major and intermediate species for burning dimethyl ether alternative diesel fuels. Both instantaneous and mean compositional structures were examined in these studies to better understand the flames.

Computationally intensive direct numerical simulation (DNS) technique which provides detailed information on turbulent reacting flows has also been used for one-point scatter data analysis. For example, early stage DNS studies of Mahalingam et al. [15] and Montgomery et al. [16] analysed turbulent non-premixed scatter data for several important combustion variables such as temperature, scalar dissipation rate and mass fraction of species using reduced kinetic mechanisms. The one-point data analysis of triple flames in an $H_2$/air mixing layer is performed using DNS [17], while heat and chemical reaction analysis using scatter data was also reported [18]. The sooting ethylene non-premixed flame was examined by employing one-point DNS [19,20] which demonstrated the importance of unsteady and multi-dimensional effects on soot formation. In addition, one-point DNS data analysis has been used for the investigation of flame-wall interactions which include basic information on the interaction of non-premixed flames with cold wall surfaces [21] and the interaction of a premixed $H_2$/air flame with an isothermal solid surface [22].

The results obtained from one-point analysis have not only provided data for comparison and validation but also raised issues relevant to local unsteady flame behaviour such as local extinction, re-ignition, blow-off, flame stabilisation and chemical equilibrium. However, the main objectives of many one-point scatter data analysis involved in experimental and computational campaigns were to study the interaction between turbulence and chemistry in non-premixed combustion with very limited work focused on compositional structures for near-wall combustion. The behaviour of the compositional structures in the near-wall region has not been completely understood because accurate flame measurements in the near-wall region are very challenging and complicated in experimental studies. However, near-wall combustion is relevant to almost all practical combustion applications. With the availability of increasing computing power, there is a large possibility of employing DNS technique to investigate compositional structures of near-wall reacting flow and thus generate a detailed database for such a problem using very large-scale massively parallel computations. DNS of $H_2$-enriched syngas flames with respect to near-wall compositional analysis, however, still represents a challenge, not only because of the broad range of scales involved but also the complexity in mixing and flame chemistry associated with the fuel variability. Depending on the $H_2$ percentage in the syngas mixture, important physical aspects relevant to high diffusivity of $H_2$ such as preferential diffusion must be considered which inevitably increase the complexity of the mathematical formulation.

**Table 1 – Fuel composition, stoichiometric mixture fraction and grid resolution for the three simulated flames.**

| Flame | $H_2$ vol% | CO vol% | $Z_{st}$ | Adiabatic flame temperature (K) |
|---|---|---|---|---|
| H | 100 | 0 | 0.028 | 2637 |
| HCO1 | 70.3 | 29.7 | 0.124 | 2430 |
| HCO2 | 33.4 | 66.6 | 0.220 | 2344 |

The objective of this work was to provide a comprehensive analysis on compositional structures and their role in the near-wall region for $H_2$ and $H_2$/CO syngas non-premixed combustion using DNS technique. In the present study, DNS results obtained by Ranga Dinesh et al. [23] were analysed with respect to flame compositional structures for an impinging jet flame configuration. The intention of this work is twofold: (1) firstly, to map the scattered structures of major, minor and radical species concentrations of $H_2$-enriched syngas non-premixed flames using DNS technique and detailed chemical kinetic mechanism including the preferential diffusion effects; and (2) to provide information on their local behaviour in the near-wall region. This work represents the first compositional analysis of major, minor and radical species of $H_2$-enriched syngas non-premixed flames with wall boundary effects using DNS technique and detailed chemistry [24] with the consideration of preferential diffusion. The remainder of this paper is organised as follows: Section 2 gives an overview of the DNS solver and the computational cases. Section 3 discusses the results in the context of major, minor and radical species distributions using one-point data analysis. Finally, Section 4 summarises the key findings and recommends some further work.

## 2. DNS solver and the computational cases

The three-dimensional DNS code solves the non-dimensional continuity equation, Navier–Stokes momentum equations, the energy equation, and the transport equations of mixture fraction and progress variable together with auxiliary equations such as the state equation for a compressible reacting gas mixture [23,25]. The non-dimensionalisation is conducted with reference to fluid properties in the fuel stream. To account for preferential diffusion, a model has been implemented in the transport equations of progress variable [23]. The code solves the equations with a fully explicit low-storage third-order Runge-Kutta scheme [26] for time integration, and a sixth-order accurate compact finite difference (Padé) scheme [27] for spatial differentiation. The studied