

Numerical Investigation of Turbulent Lean Premixed H₂/CO Combustion at Elevated Pressures

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1 Introduction

The use of hydrogen-rich syngas fuels as a supplement for petroleum fuels offers the advantage of a low carbon fuel without significantly changing the current combustion technologies and the associated massive infrastructure [1]. In this context, combustion of high-hydrogen content (HHC) syngas fuel with a broader reaction class such as significant quantities of hydrogen diluted with carbon monoxide is undoubtedly significant [2]. Particularly, turbulent lean premixed combustion characteristics of HHC fuels at elevated pressures is of both fundamental and practical importance for clean and efficient next generation combustion engines [3]. Recently, Direct Numerical Simulation (DNS) calculations have certainly added a great deal of understanding, providing valuable insights to many issues such as preferential diffusion effects [4], local flame propagation [5] and flame stretch [6] in turbulent lean premixed combustion benchmark problems. Although previous DNS studies with simple finite-rate and complex detailed chemistry provide valuable insights into structure and propagation of turbulent lean premixed combustion of hydrogen and hydrogen blended alternative fuel at atmospheric pressure, DNS investigation focus on flame structure and propagation of lean premixed hydrogen and/or hydrogen-rich alternative fuel combustion at elevated pressures are performed seldomly in the past.

There are several unresolved issues outstanding for DNS of turbulent lean premixed combustion at elevated pressures, which need further investigation. For example, majority of detailed chemical kinetic mechanisms which have been used in DNS of lean premixed hydrogen or hydrogen-enrich syngas combustion are mostly validated only at atmospheric pressure. Very recent studies reported hydrogen and HHC fuel chemical kinetic mechanisms at elevated pressures, for example [7]. Therefore, it is still not clear how important the role of detailed chemical mechanisms in predicting DNS based key chemical species mass fractions such as H, OH and HO₂ in lean premixed combustion at elevated pressure. Furthermore, it is also not clear how important the role of preferential diffusion on predicting flame wrinkling and heat release rate of HHC lean premixed syngas flame at elevated pressures.

The present study has two principal aims. The first is to investigate the impact of detailed chemical kinetic model employing in DNS on prediction of species mass fractions of lean premixed HHC H₂/CO syngas turbulent flame at elevated pressure. For this, we compare contour distributions and conditional mass fractions of radical species such as H, OH and CH₂O between two H₂/CO syngas

chemical kinetic mechanisms. The second aim is to study the preferential diffusion (non-unity Lewis number) effect on flame structure and propagation of lean premixed HHC H₂/CO syngas turbulent flame at elevated pressure. For this, we present temperature contours and scattered data of heat release rates.

2 Mathematical Formulation

In the context of experimental investigation of flame structure and propagation of turbulent premixed combustion at elevated pressure, two commonly-used turbulent premixed flame geometries, Bunsen-type flames and centrally-ignited outwardly propagating (expanding spherical) flames have been studied extensively, for example [8,9]. In this work, we attempt to find solutions to aims noted above based on DNS of centrally-ignited outwardly propagating lean premixed HHC syngas flames. In all test cases, two-dimensional DNS were performed for HHC lean premixed H₂/CO syngas fuel mixture with 70% of H₂ and 30% of CO by volume with an equivalence ratio of 0.7. The centrally-ignited outwardly propagating lean premixed HHC syngas flames have been simulated using DNS incorporating detailed chemistry and multicomponent diffusion transport models. The time-dependent compressible DNS code *ParComb* [10] solves the continuity equation, Navier-Stokes momentum equations, the energy equation, species balance equations together with auxiliary equations such as the state equation. In this study an equation is solved explicitly for each and every chemical species with comprehensive detailed chemistry, simultaneously with the Navier-Stokes equations. We also employed multicomponent diffusion transport models to compute the diffusive processes. The diffusion velocity of each species is calculated using multi-species diffusion coefficient matrix including binary diffusion and Soret effects. We have employed two H₂/CO syngas chemical kinetics mechanisms. The first detailed mechanism employed is the H₂/CO kinetic scheme developed by Mass and Pope [11]. This reaction model involves 13 species (CO, HCO, CH₂O, CO₂, H₂O, O₂, O, H, OH, HO₂, H₂O₂, H₂, N₂) and 67 individual reactions, but only validated at the atmospheric pressure. The second mechanism used in this study is the H₂/CO kinetic scheme developed by Goswami et.al. [7]. This reaction model incorporates the thermodynamic, kinetic, and species transport properties related to elevated pressure H₂ and CO oxidation, consisting of 16 species (CO, HCO, CH₂O, CO₂, H₂O, O₂, O, H, OH, HO₂, H₂, N₂, HE, AR) and 52 individual reactions.

We used a square box which has a length of 1.5×10^{-2} m on each side. The grid resolution was equal to $\Delta x = 9 \times 10^{-6}$ m, resulting in 1600 and 1600 computational nodes respectively along each spatial direction. A time step of approximately 1.8×10^{-9} s was used for all simulations. The equations are discretised in space on a two-dimensional Cartesian grid with high-order finite difference numerical schemes. Derivatives are computed using centered explicit schemes of order six except at boundaries where the order is progressively reduced to four. Temporal integration is realized with a Runge–Kutta algorithm of order four. A Courant-Friedrichs-Levy (CFL) condition for the convective terms and a Fourier condition pertaining to the diffusion terms are treated to ensure the stability of the explicit integration and determine a suitable time step. To maintain the constant pressure throughout the simulation, boundary conditions are treated with the help of improved non-reflecting inflow/outflow Navier-Stokes characteristics boundary condition (NSBC) by considering additional terms in the definition of the wave amplitudes, and the relaxation treatment for the transverse gradient terms in analogy with the pressure relaxation. The initial Gaussian temperature profile has been constructed to mimic spark ignition of the mixture using a Gaussian temperature profile. The initial isotropic turbulent velocity field for each case was initialised using a combined approach of digital filtering (DF) and random noise diffusion. An initial temperature of $T_u = 300$ K is uniformly distributed across the entire domain.

3 Results and Discussion

3.1 Influence of Chemistry on Prediction of Species Mass Fractions at Various Pressures

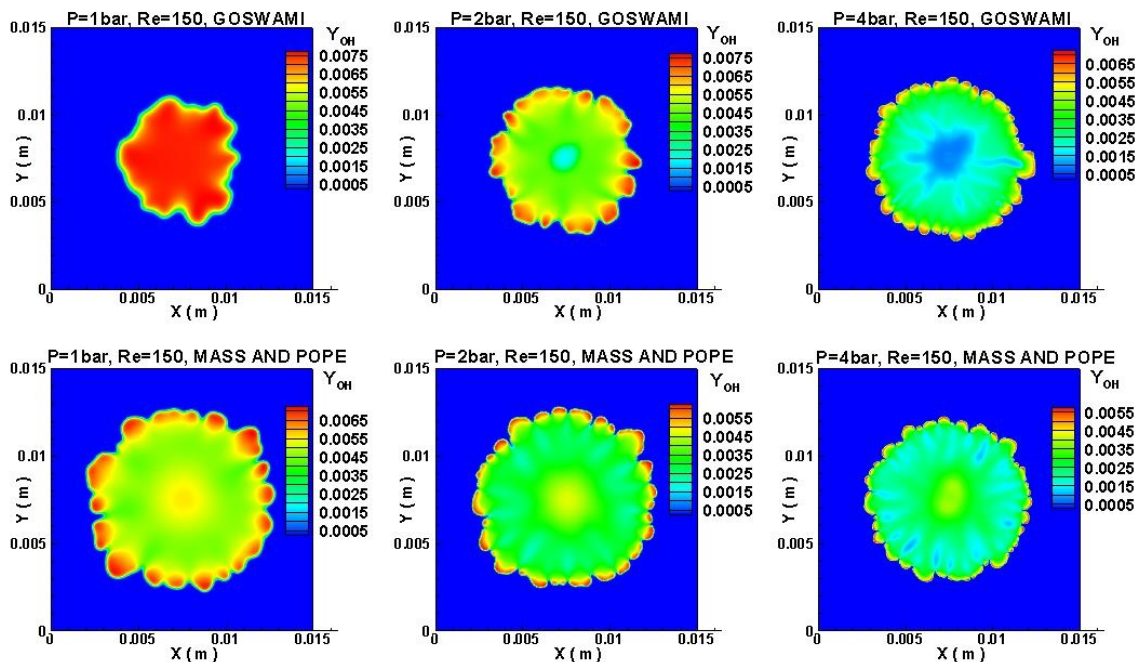


Fig.1. Contours of instantaneous mass fraction of OH obtained using chemical mechanism of Goswami et. al. [7] (top) and Mass and Pope [11] (bottom) at constant turbulent Reynolds number of $Re_t=150$ and at constant pressure values $p=1\text{bar}$, 2bar and 4bar .

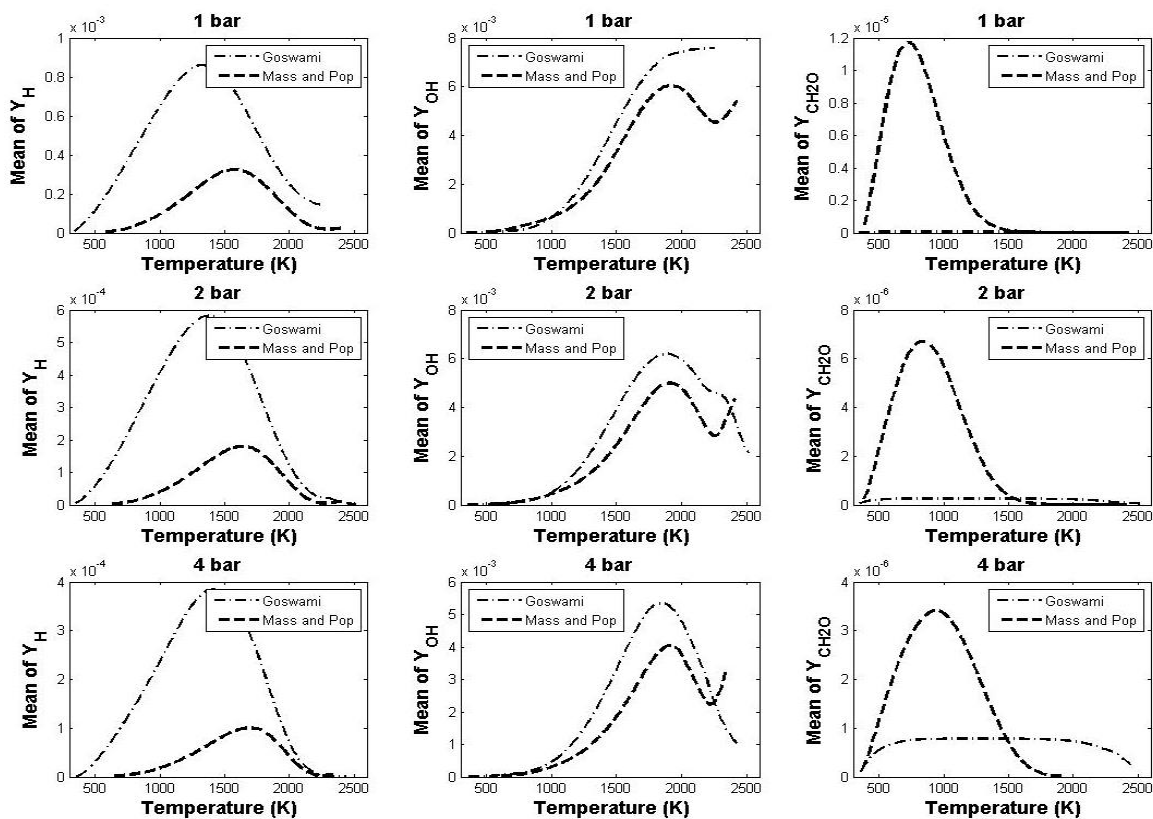


Fig.2. Conditional mean values of mass fractions of H radical, OH radical and CH_2O radical as a function of temperature obtained using chemical mechanism of Goswami et. al. [7] and Mass and Pope [11] at constant Reynolds number of $Re_t=150$ and at constant pressure values of $p=1\text{bar}$, 2bar and 4bar .

To compare the prediction of radical species mass fraction distribution between two chemical kinetics mechanisms at different pressure levels, six DNS simulations at different pressure levels with the inclusion of non-unity Lewis numbers were performed by employing detailed chemical mechanism of Goswami et.al. [7] and Mass and Pope [11]. In the present study, three different pressure values of $p=1\text{bar}$, 2bar and 4bar at constant turbulent Reynolds number of $Re_t=150$ were considered.

Fig. 1 displays contour plot of instantaneous mass fraction of OH radical at different pressure levels of $p=1\text{bar}$, 2bar and 4bar and constant turbulent Reynolds number of $Re_t=150$. Comparison between two chemical mechanisms shows common features for mass fraction of OH radical at different pressure levels of $p=1\text{bar}$, 2bar and 4bar . To further identify impact of pressure on radical species formation, Fig.2 shows the conditional mean values of mass fractions of H, OH and CH_2O as a function of temperature at pressure levels 1bar , 2bar and 4bar . Conditional plots of OH show no significant differences between two mechanisms at different pressure levels, but conditional plots of H and CH_2O display large differences between two chemical kinetics mechanisms at all pressure level, with the disagreement becoming stronger at higher pressure. We also observed that conditional plot of HO_2 indicates similar trends as CH_2O between two mechanisms at all pressure levels (not shown in Fig.2).

3.2 Effects of Preferential Diffusion on Flame Structure at Elevated Pressure

To compare the results between non-unity Lewis number and unity Lewis number at elevated pressure, one DNS test case with non-unity Lewis number and another DNS test case with unity Lewis number were performed at elevated pressure value of $p=4\text{bar}$, and at turbulent Reynolds number of $Re_t=150$ by employing the detailed chemical mechanism of Goswami et. al. [7].

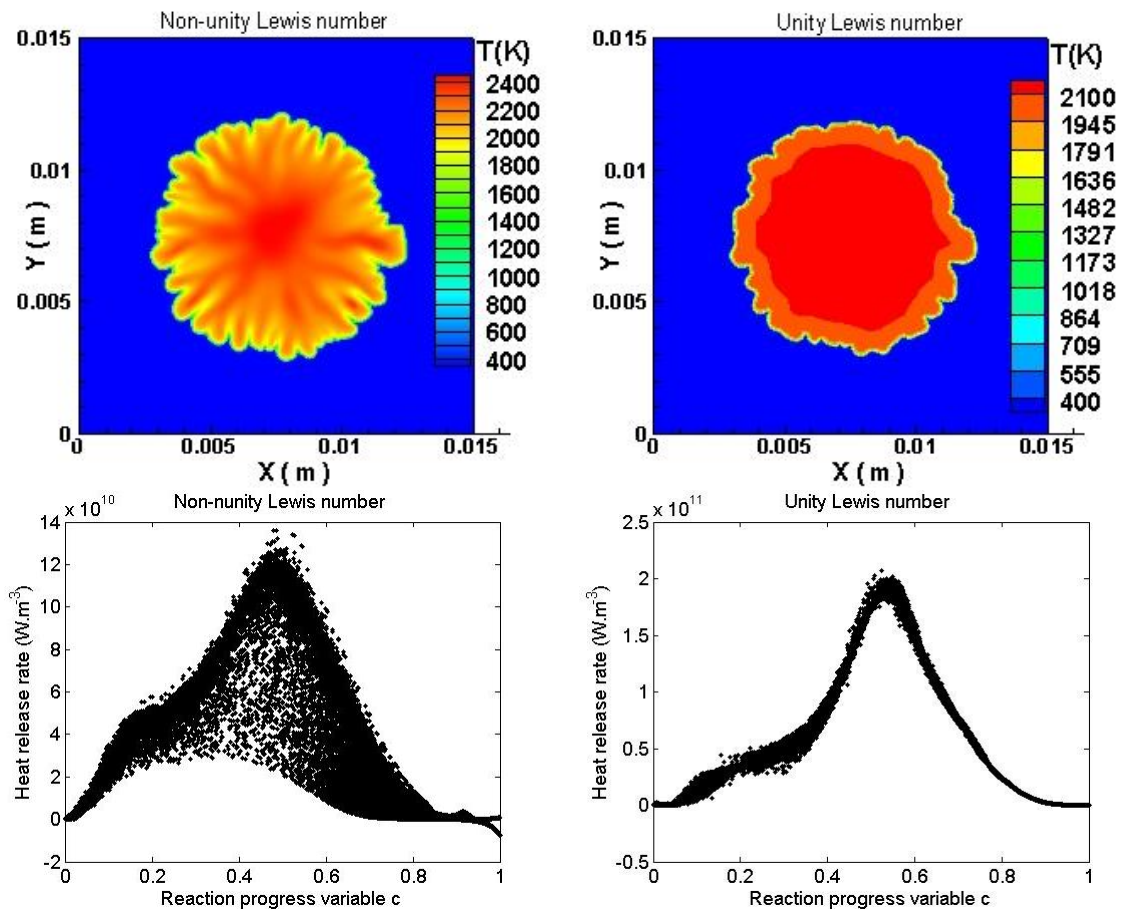


Fig. 3. Top: Contours of instantaneous flame temperature; Bottom: Scatterplots of heat release rate with non-unity Lewis number (left hand side) and with unity Lewis number (right hand side) at constant turbulent Reynolds number of $Re_t=150$ and at constant pressure of $p=4\text{bar}$.

Fig. 3 shows comparison of instantaneous snapshot of flame temperature and scattered heat release rate between the non-unity Lewis number case and the unity Lewis number cases at constant elevated pressure value of $p=4\text{bar}$ and constant turbulent Reynolds number of $Re_t=150$. Fig.3 exhibits local increase or reduction of the flame intensity with strong diffusional-thermal cellular instability in the non-unity Lewis number case as a result of significant change of total enthalpy in the gas mixture compared to the unity Lewis number case which is expected to have hydrodynamic cellular instability. Since H_2 atom is present in large concentration in these flames, its contribution to the total enthalpy of the mixture is significantly contributing to the flame temperature. It is seen from the unity-Lewis number case that the reaction zone is insensitive to steady straining in the absence of non-unity Lewis number at elevated pressure. This confirms that the strain rate effects remain closely tied to non-unity Lewis number and preferential diffusion effects at elevated pressure value of $p=4\text{bar}$. As seen in Fig. 3, the scatter of heat release rate display two differences: (1) the peak heat release rate of the non-unity Lewis number case is about $1.4 \times 10^{11} \text{ (Wm}^{-3}\text{)}$, while its value for the unity Lewis number case is about $2.5 \times 10^{11} \text{ (Wm}^{-3}\text{)}$; (2) the scatter of the unity Lewis number case shows more symmetric behaviour compared to non-unity Lewis number case. Furthermore, when preferential diffusion effects are neglected, the peak value of heat release rate and temperature correspond are located at the stoichiometric condition.

4 Conclusions

DNS of turbulent lean premixed high hydrogen content (HHC) H_2/CO syngas flame with detailed chemistry and multi-component transport models has been carried out for outwardly propagating spherical flames in the thin reaction zone regime. Simulations were performed for lean premixed H_2/CO syngas fuel mixture with 70% H_2 and 30% CO by volume with an equivalence ratio of 0.7. Statistics pertaining to the flame chemistry and preferential diffusion were obtained from the computed fields. In the sensitivity study of chemical kinetic mechanisms with DNS at elevated pressure, a comparison of radical species distributions between two detailed chemical reaction mechanisms at identical elevated pressures highlight key differences in radical species formations such as H , OH and HO_2 . In the preferential diffusion study case, it is found that non-unity Lewis number effects play a significant role in the local chemical reaction as well as diffusional-thermal cellular flame structure and heat release rate in the thin reaction zone at elevated pressures for turbulent lean premixed HHC H_2/CO flames.

Acknowledgments

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