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The effect of molecular diffusion on the flow field of hydrogen enriched Methane-AIR stratified swirl burner

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Abstract

This article investigates the effects of molecular diffusion and utilizing unity and specific Schmidt numbers for species on the results of the simulations, in the presence of highly mobile species H_2, in the fuel stream, while stratification and swirl are used for flame stabilization. In addition, we have characterized regions where both molecular diffusion and turbulent transport play a significant role. For this purpose, a stratified swirl burner called the Cambridge-Sandia burner will be used as a case study. A total of 40% hydrogen (on a volume of fuel basis) is added to both slots of the burner. Two models are used: (i) the Schmidt numbers for all species are equal to unity, and the Sutherland coefficients are constant for all of them, and (ii) species-specific Schmidt numbers and Sutherland coefficients are taken into account. It is investigated how different models affect various flow fields, such as velocity, temperature, and species mass fractions. The PaSR combustion model, and the SST $k-\omega$ turbulence model, are used in our computational method. It is shown that by adding hydrogen and in the presence of stratification, preferential diffusion of lighter species affect temperature, as well as H_2 mass fractions, so it cannot be overlooked. In premixed case, it has a minor influence on species concentration, but it still affects temperature distributions.

Keywords: molecular diffusion, hydrogen enrichment, stratified burner, Schmidt number

Introduction

Currently, fossil fuels meet 80% of the world's energy needs, but the pollutants they emit are hazardous to health and the environment. Several high-tech and clean combustion methods have been developed in response to strict pollution regulations, including lean premixed combustion, MILD combustion, and hydrogen-enriched fuels. Because lean premixed combustion ensures complete combustion, carbon monoxide is reduced, and, owing to lower fuel temperatures, NOx and other pollutants sensitive to high temperatures are only moderately produced. In MILD combustion, nitrogen-oxide pollution is lower, while the flame stability is higher in this combustion regime. [1].

Many parameters are affected by stratification, such as heat release, flame speed, local flame structure, combustion efficiency, and pollutant emissions. [18]. For instance laminar flame speed is increased by stratification [9]. Additionally, a stratified mixture with the same equivalence ratio exhibits a higher turbulent flame speed in a lean area than a homogeneous mixture [15]. It also enhances the mean reaction rate in lean flames [2].

Adding hydrogen to hydrocarbon fuel improves flame stability and lowers CO and UHC emissions while increasing NO_x emissions due to a higher burnt gas temperature, but this can be compensated by burning ultra-lean mixtures since hydrogen increases the lean blowout limit. [7].

Stabilizing flames by creating recirculation zones using a bluff-body and swirling flows is a commonly used method in many combustion devices [16, 19]. Also, a large number of combustion devices, such as gas turbines, aero engines, and automobile engines, are operated in inhomogeneously premixed mode, either for flame stability in globally lean combustion, or to meet practical mixing region length constraints[18]. However, since hydrogen has better flame-holding characteristics than hydrocarbon fuel [6, 12], enriching a hydrocarbon fuel with hydrogen [13] is a useful strategy for decreasing combustion instabilities under ultra-lean conditions. Due to thermal-diffusion instability, adding hydrogen to a system increases modeling complexity; hence exact numerical models are required. Numerous experiments have been undertaken to determine the impact of hydrogen addition on the stability, reactivity, and pollutant emissions of methane-air flames [10-12, 21].

The addition of 20% H_2 to CH_4 in the Darmstadt flame series has been demonstrated to modify differential H_2 diffusion, revealing that stratification levels have no effect on CO levels but change H2 distribution. [24]. Based on these results, Wen et al. [28] used a flamelet approach to analyze the flame structure by considering molecular diffusion and stretch effects. The results demonstrate that as turbulent mixing grows, differential diffusion becomes less critical, and the unity Lewis number assumption performs as well as mixture-averaged and multi-component models in these situations [28].

Mardani et al. [20] compared molecular diffusion to turbulent diffusion using bimolecular and multicomponent models, proving that molecular diffusion is crucial in flameless combustion.

In contrast to turbulent flow, where turbulent transport is dominant, in reacting turbulent flow, turbulent transport and molecular diffusion are comparable, so neither can be overlooked because the heat released by the combustion (turbulence, combustion interaction) expands the flow field and reduces the vorticity [14], which is the result of density drop along the flame front, which can drop by six to seven times [17].

Salavati-Zadeh et al. [23] investigated the influence of molecular diffusion and variations in the Schmidt number of various species on model accuracy in the flameless regime, finding that molecular diffusion does not affect the findings if appropriate Schmidt numbers are not used for each species. In flameless regimes, temperature and OH mass fractions can be well predicted by adding molecular diffusion, but the effects of molecular diffusion vanish in conventional combustion regimes.

In order to validate the utilized numerical method an experimental results are needed .The Cambridge-Sandia stratified swirl burner has created an extensive database [22, 23]. In this burner, premixed mixtures with different equivalence ratios of fuel and air flow through two annular inlets (to generate different stratification ratios SR=ϕ_i / ϕ_o). Besides An air co-flow is also present to avoid atmospheric air entertainment. In conjunction with the swirling flow in the outer slot, the central bluff body stabilizes the flame, producing a recirculation zone. The swirl number (Sw) is the ratio between tangential and axial velocities.

The primary goal of this research is to find out how molecular diffusion affects the structure of hydrogen-enriched stratified flames and whether if the addition of molecular diffusion into governing equations affects the flow field, temperature, and species mass fractions or not. Currently, only a limited number of papers have examined the effect of differential diffusion in stratified burners, and the effect of considering different Schmidt numbers versus unity Schmidt numbers for every species has not been considered in a hydrogen-enriched stratified Cambridge-Sandia burner. The authors employ open-source CFD software OpenFOAM to examine a stratified hydrogen/methane/air flame. Model validation is done using methane/air combustion and hydrogen is added to the fuel stream. The effects of two different models on flame structure, temperature, and species mass fraction are then investigated.

Burner configuration

Figure 1 shows the burner geometry schematically. It is possible to adjust the equivalence ratio of each slot independently in order to create flames of differing stratification ratios. Only two cases shown in Table 1 will be investigated in this study. The velocities of the outer slot, inner slot, and co-flow are constant in all cases and are 8.31, 18.7, and 0.4, respectively. Two simulations with different models have been conducted in both cases, as mentioned previously. During the addition of hydrogen, the velocity of premixed mixtures entering from slots and the global equivalence ratio is kept constant. The density and mass flow rate of fuel decrease as hydrogen is added.

Numerical procedure

The Favre-averaged equations of continuity, momentum, energy, and species are used as flow equations. Using the open-source CFD code OpenFOAM, Reynolds Averaged Navier-Stokes (RANS) based simulations are performed. The turbulent viscosity in the momentum equations is calculated using SST $k-\omega$ turbulence model adopted with wall. In this study, a reduced mechanism including 15 species and 57 reactions proposed by Valorani et al. [26], has been used to characterize the flame structure, temperature, and major species.

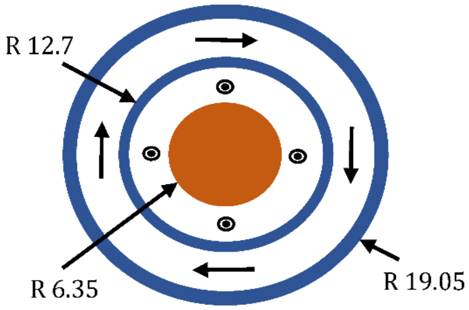


Figure 1. The top view of the stratified swirl burner (SwB) [25]. All dimensions are in mm.

Table 1. The selected operating conditions

Flame	Sw	ϕ_i	ϕ_o	case
SwB2	0.45	0.75	0.75	premixed
SwB6	0.45	1	0.5	stratified

As in previous studies, radiation heat transfer is neglected [22]. A molecular diffusion term is included in the species transport equation using the OpenFOAM code, incorporating different and constant Schmidt numbers for each species, as shown in Equation 1.

$$\frac{\partial}{\partial t}\left(\bar{\rho}\tilde{Y}_k\right)+\frac{\partial}{\partial x_j}\left(\bar{\rho}\tilde{Y}_k\tilde{u}_j\right)=\frac{\partial}{\partial x_j}\left(\left(\frac{\mu}{Sc_k}+\frac{\mu_t}{Sc_k^t}\right)\frac{\partial\tilde{Y}_k}{\partial x_j}\right)+\tilde{\omega}_k \qquad (1)$$

s = 1, …, n

In Equation 1, μ, and μ_t, respectively, are laminar and turbulent dynamic viscosities, while Sc_s and Sc_s^t represent Schmidt number of specie k and turbulent Schmidt number, respectively. The values of Sc_s were taken from Ref. [23] while, Sc_s^t is assumed to be equal to 0.7 throughout all the simulations.

A finite volume approach is used to discretize the governing equations. The standard central scheme is used to discretize diffusion terms. For accuracy and stability, we use second-order TVD schemes for discretizing convection terms. To solve pressure-velocity coupling the PISO algorithm was used.

In a similar way to previous works [5, 8, 27], two criteria have been implemented to ensure convergence. In the first, the residual of all variables must be less than 10^{-6} at each time step. Second, at a section near the outlet (10% to exit plane), the average temperature should not vary by more than 1K or maximum velocity should not differ by more than 0.1.

3D computational domain (shown in Figure 2) is a cylindrical region of diameter (200 mm) and length of (300 mm) according to Ref. [4].

SwB2 case was simulated using three different grids to ensure the results were independent of the grid. The grid with 160000 cells makes up the base mesh (coarse). There are no significant deviations in Figure 3 with 470000 cells (average) and 800000 cells (fine). As a result, we selected a grid number of 470000 cells to reduce computing costs during simulations of this study. For the boundary conditions, at the inlet of both slots, the temperature, velocity components (tangential and axial), and mixture compositions are constant. The zero velocity and no heat transfer conditions are applied to all walls. For far-field and outlet, zero-gradient is applied to all variables except pressure which is equal to atmospheric pressure.

Results and discussion

The comparison of computational results and experimental measurements [25, 29] are carried out for SwB6 case in order to validate the mathematical model. In Figure 4, the tangential and axial components of velocity, temperature, and CO_2 mass fraction at different cross-sections are compared with experimental results for both models. There is a good agreement between the simulation results and experimental measurements. The ratio between turbulent and molecular viscosity (RTMV) is shown in Figure 5 to gain insight into the regions of the domain where differential diffusion and turbulent transport are comparable. The region of importance for molecular and turbulent transport is much larger in the stratified case (SwB6) without hydrogen addition than in the premixed case (SwB2). The region with RTVM less than ten increases, particularly in the axial direction, when hydrogen is added. Hence, the effect of differential diffusion in pure methane cases may be more pronounced in stratified case, particularly in regions far from the burner exit, but by adding H_2, it might be significant in stratified and premixed cases as well. To quantitatively investigate this parameter, radial profiles of RTMV in different cross-sections, and on the centerline have been depicted in Figure 6.

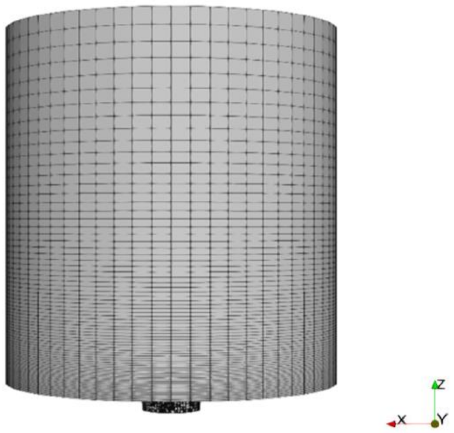
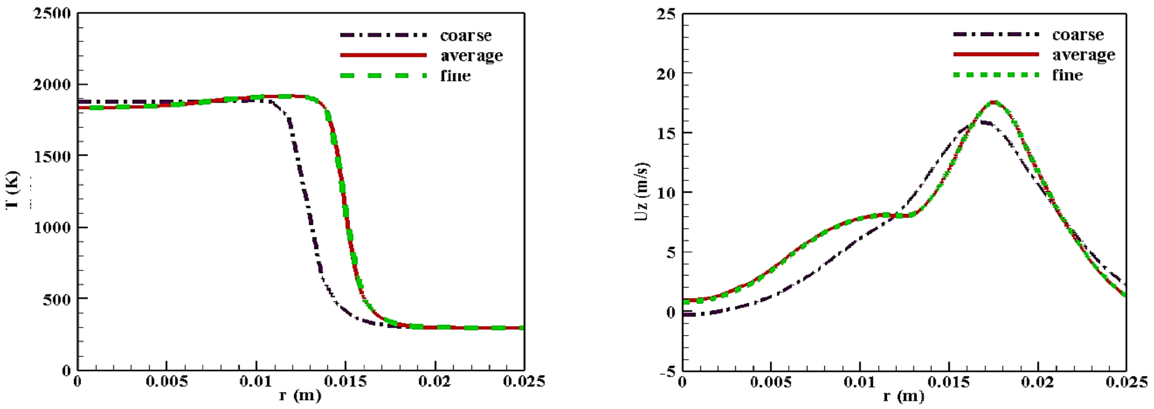


Figure 2. The computational grid used in this study



a

b

Figure 3. Grid independence check. Temperature profile (a) at section (z = 40 mm) and axial velocity profile (b) at section (z = 30 mm) using three distinct cell numbers.

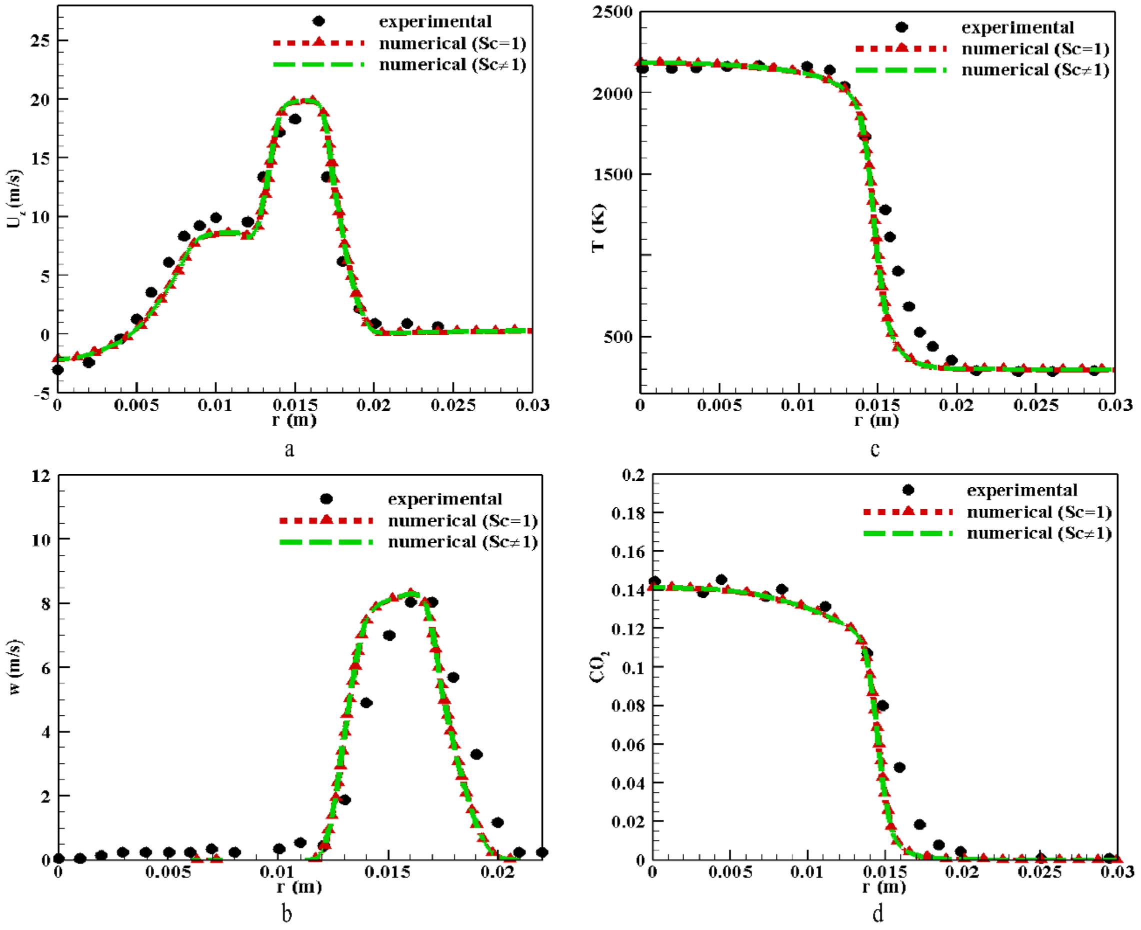


Figure 4. Comparison between experimental measurements [25, 29], and computations for SwB6. Profiles at YZ plane. (a) Axial velocity, (b) swirling velocity, (c) temperature, (d) CO_2 mass fraction. At cross sections: z = 40 mm (right column), z = 10 mm (left column)

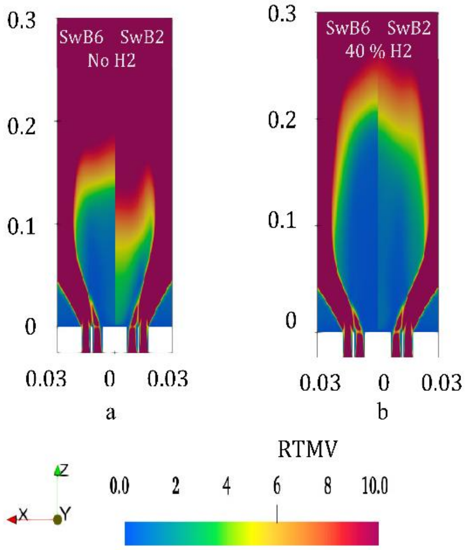
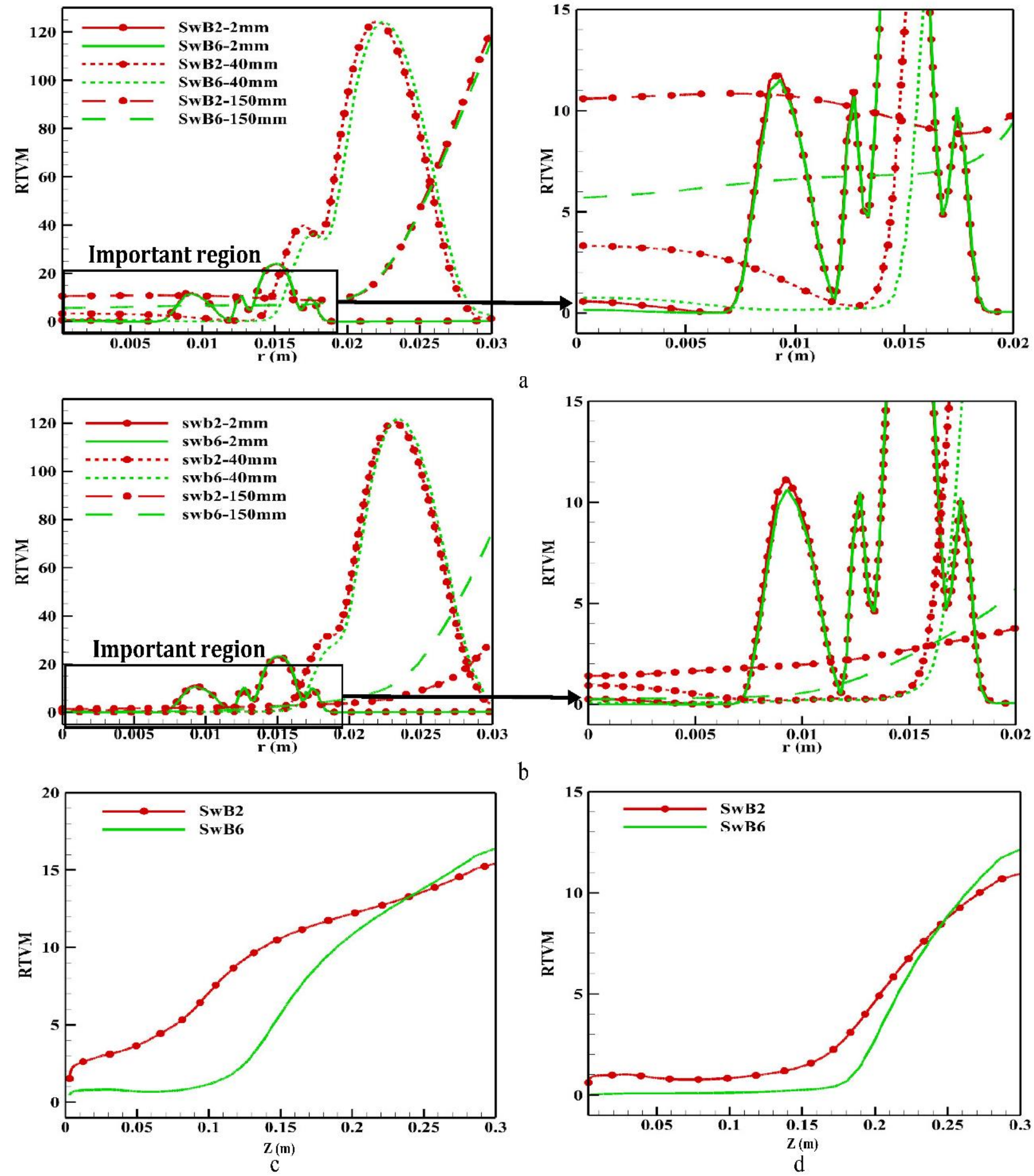


Figure 5. The contours of the ratio between turbulent and molecular viscosity (RTMV) for premixed (SwB2) and stratified (SwB6) cases. Pure methane as fuel (a) hydrogen enriched methane (b).

It can be seen in figure 6 that molecular diffusion plays an important role in some regions. These regions are caused by turbulence and combustion interactions and the relaminarization process. According to Figure 6 by increasing hydrogen concentration, differential diffusion becomes more significant in a wider area, both radially and axially.

Some important factors about the simulated cases are worth mentioning, which can affect molecular diffusion. Firstly, RTVM in stratified cases, is always less than premixed cases, especially in pure methane burning; therefore, molecular diffusion is expected to have a more significant impact in stratified cases. Secondly, a vital flow characteristic in swirl bluff-body stabilized burners is the recirculation zone volume and strength. It has been observed that stratified case (SwB6) exhibits a smaller recirculation zone than premixed case (SwB2). Simulated results showed the same effect, and both stratified and premixed cases showed a reduction of recirculation zones with H_2 added (not shown here). There is an important role for this region since the residence time is longer there, and it has been demonstrated that this region can amplify the effects of molecular diffusion [3]. Since the recirculation zone in the SwB2 case is more prolonged and stronger, it is anticipated that light molecules and mobile molecules will diffuse out of this region due to thermal expansion and a longer residence time.



a

b

c d

Figure 6. Radial profiles of RTVM at different cross-sections. Pure methane (a) hydrogen enriched methane (b) and axial profiles of RTVM. Pure methane (c) hydrogen enriched methane (d).

Thirdly, because of the richer inner slot in stratified cases, there is a higher temperature, and the molecules have more kinetic energy, promoting diffusion. Additionally, the higher temperature and heat release enhance the relaminarization effect, further improving diffusion. Finally, the inner slot of the stratified case is richer so that H_2 availability is higher, causing a steep concentration gradient that is a stimulant to diffusion. Keeping these points in mind, the simulation results for temperature, H_2, OH, CO, and CO_2 are depicted in the subsequent parts.

Figure 7 illustrates the temperature profiles in different cross-sections. Based on this figure, it can be seen that simulations result in a higher temperature when molecular diffusion is taken into account regardless of the stratified or premixed cases. It is noteworthy that when considering molecular diffusion, the flame does not expand radially in cross-sections near the burner exit, while it does in downstream locations (z = 150 mm).

In order to understand how molecular diffusion affects temperature, radial profiles of OH radical, as an indicator of reaction zone, and H_2, as a highly mobile specie, are depicted in Figure 8 and figure 9, respectively.

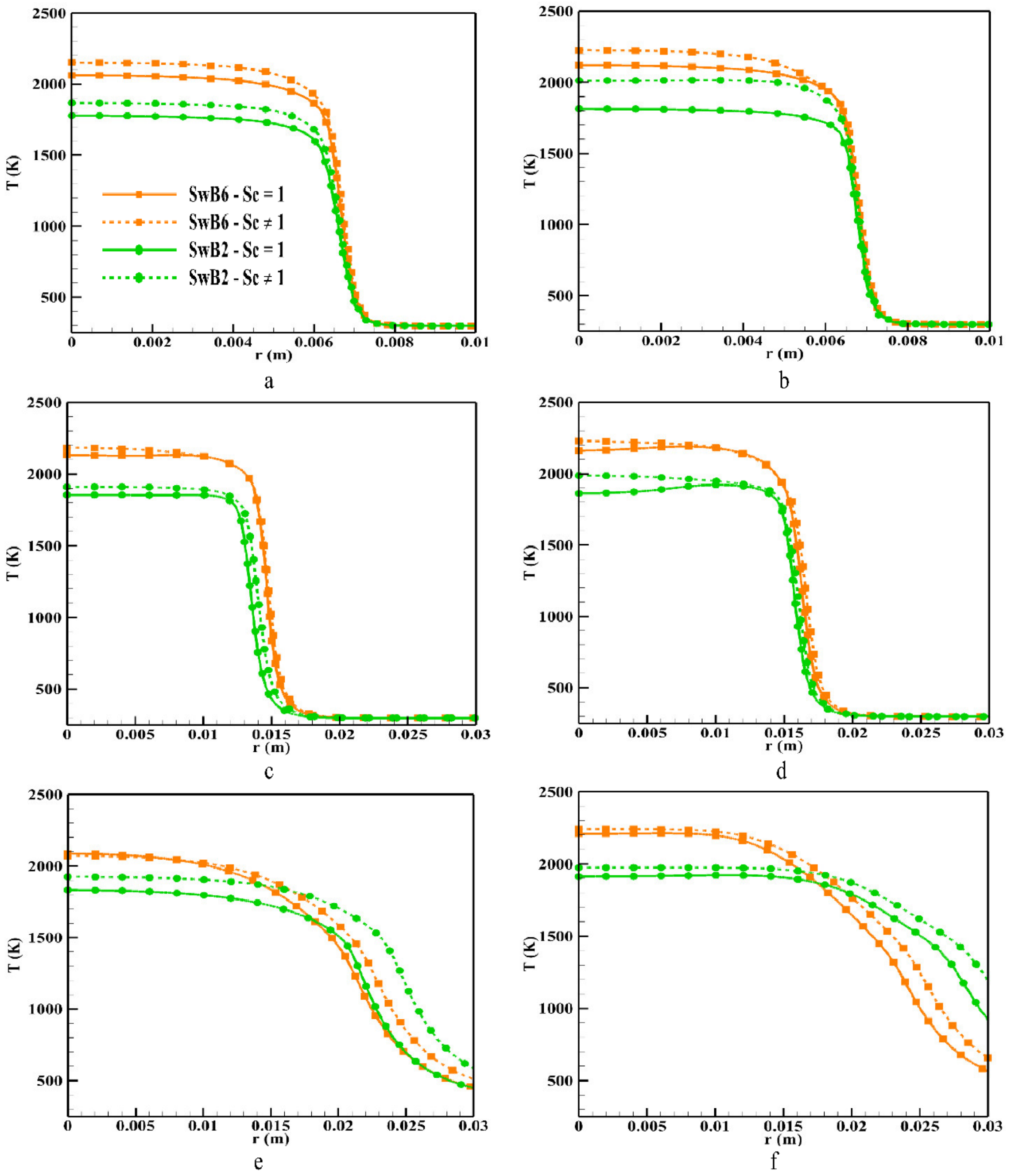
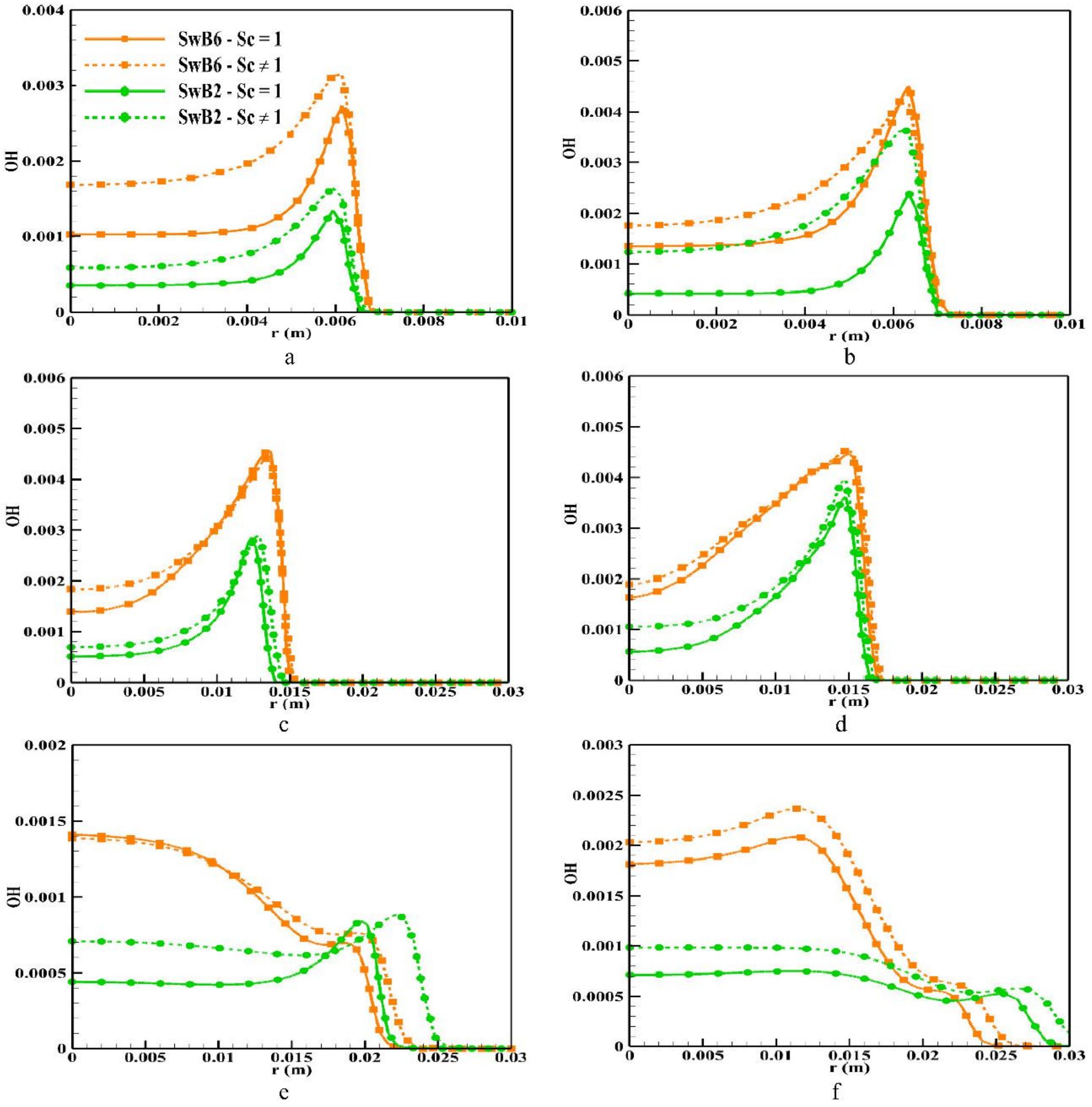


Figure 7. Temperature profiles at different cross sections. 2mm (top row) 40mm (middle row) 150mm (bottom row). Pure methane as fuel (left column) 40% hydrogen (on the volume of fuel basis) added to fuel stream (right column).

Figure 8 shows an increase in OH mass fraction in all cross-sections in both premixed and stratifies cases in pure methane/air and methane-H_2/air burning. Comparatively to downstream sections, the mass fraction of OH increases more near burner exit (2 mm). A radial expansion of OH profiles in downstream sections indicates an expansion of reaction zones. Figure 9 illustrates the H_2 mass fraction in different cross-sections. Molecular diffusion affects the mass fraction of H_2 since it is mobile and light. Taking molecular transport into account, while burning pure methane results in a lower amount of H_2 in all cross-sections, which is attributed to molecular diffusion. As hydrogen is just produced in the reaction zone, it diffuses radially outward, so there is a slight expansion in radial distribution and a reduction in peak value. Because of the high concentration in unburned reactants, H_2 diffuses into the reaction zone which agrees with the results of Schneider et.al. [24]. Therefore, the mass fraction of hydrogen near the centerline (the core of the reaction zone) near the burner exit in the stratified case increases.

It is unclear why, in the premixed case, even after adding H_2, molecular does not affect the mass fraction of light species like hydrogen, whereas in the stratified case, it does. This is presumed to result from a back-supported flame in stratified cases. As the inner slot is rich, more hydrogen is produced here. This effect is evident in cases without hydrogen addition (Figure 9 (a, c, e)). In addition, the recirculation zone in the premixed case is larger, so light species have more time to diffuse out of the zone. For a detailed understanding of this issue, more research is still needed.



a b c d e f

Figure 8. Comparison of OH mass fraction using different models for premixed and stratified case. 2mm (top row) 40mm (middle row) 150mm (bottom row). Pure methane as fuel (left column) 40% hydrogen (on the volume of fuel basis) added to fuel stream (right column).

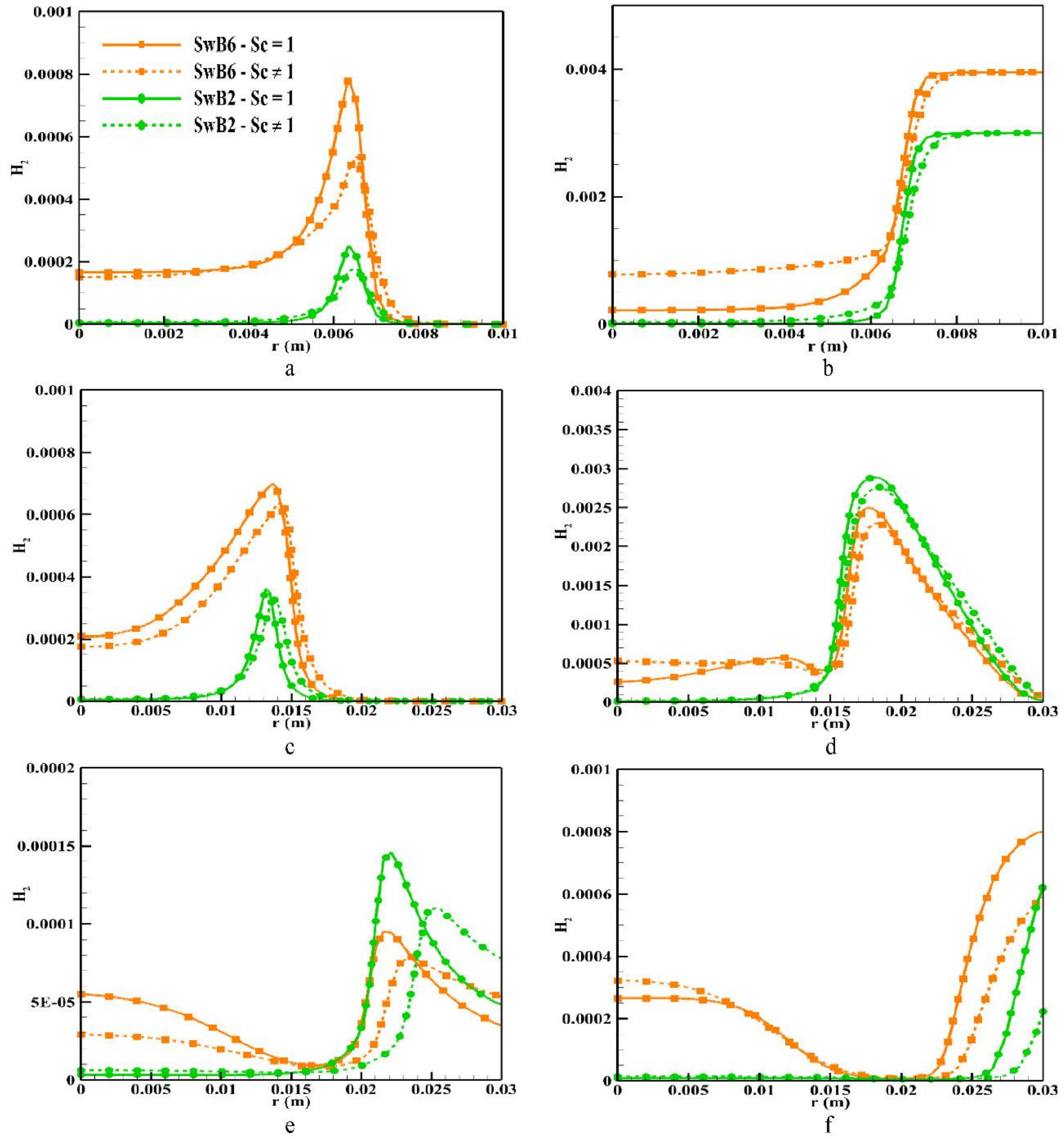


Figure 9. Comparison of H_2 mass fraction using different models for premixed and stratified case. 2mm (top row) 40mm (middle row) 150mm (bottom row). Pure methane as fuel (left column) 40% hydrogen (on the volume of fuel basis) added to fuel stream (right column).

Conclusions

A stratified burner was studied in this paper using two different molecular diffusion models in species transport equations. In the first model, the Schmidt numbers for all species and flow were equal to one. While in the second model, the Schmidt numbers were specific and constant. Additionally, viscosity was computed using constant values in the Sutherland formula in the first model. While in the second model, like Schmidt numbers, the constant values in Sutherland equations are unique for each species. In order to investigate the effects of molecular diffusion in stratified and premixed combustion, especially when the fuel is enriched with H2, two cases of Cambridge- Sandia burner were examined, a premixed case (SwB2) and a stratified case (SwB6).

The results revealed that taking molecular diffusion into account results in computing a higher temperature in all cases and cross-sections. However, interestingly in the premixed case, there was no preferential diffusion in contrast to the stratified case. To understand the zones where laminar viscosity and turbulent viscosity are comparable, the ratio between these variables was computed, showing that adding hydrogen makes laminar viscosity important in premixed and stratified cases, but all in all, it is more important in the stratified case. Many parameters, including laminar viscosity, availability of hydrogen, relaminarization, recirculation zone, residence time, and thermal expansion, can affect molecular diffusion; so to understand which is dominant, detailed simulations using LES or DNS are needed.

References

[1] Abuelnuor, A., et al., 2014, "Flameless combustion role in the mitigation of NOX emission: a review". International journal of energy research, 38(7): p. 827-846.

[2] Anselmo-Filho, P., et al., 2009, "Experimental measurements of geometric properties of turbulent stratified flames". Proceedings of the Combustion Institute, 32(2): p. 1763-1770.

[3] Barlow, R.S., et al., 2012, "Effects of preferential transport in turbulent bluff-body-stabilized lean premixed CH4/air flames". Combustion and Flame, 159(8 :(p. 2563-2575.

[4] Brauner, T., W. Jones, and A. Marquis, 2016, "LES of the Cambridge Stratified Swirl Burner using a Sub-grid pdf Approach". Flow, Turbulence and Combustion, 96(4): p. 965-985.

[5] Christo, F.C. and B.B. Dally, 2005, "Modeling turbulent reacting jets issuing into a hot and diluted coflow". Combustion and flame, 142(1-2): p. 117-129.

[6] Day, M.S., X. Gao, and J.B. Bell, 2011, "Properties of lean turbulent methane-air flames with significant hydrogen addition". Proceedings of the Combustion Institute, 33(1): p. 1601-1608.

[7] Do Sacramento, E., et al., 2008, "A hydrogen energy system and prospects for reducing emissions of fossil fuels pollutants in the Ceará state—Brazil". International Journal of Hydrogen Energy, 33(9): p. 2132-2137.

[8] Fordoei, E.E., K. Mazaheri, and A. Mohammadpour, 2021, "Effects of hydrogen addition to methane on the thermal and ignition delay characteristics of fuel-air, oxygen-enriched and oxy-fuel MILD combustion". International Journal of Hydrogen Energy, 46(6 :(8p. 34002-34017.

[9] Galizzi, C. and D. Escudié, 2010, "Experimental analysis of an oblique turbulent flame front propagating in a stratified flow". Combustion and flame, 157(12): p. 2277-2285.

[10] Gauducheau, J., B. Denet, and G. Searby, 1998, "A numerical study of lean CH4/H2/air premixed flames at high pressure". Combustion Science and Technology, 137(1-6): p. 81-99.

[11] Guo, H., et al., 2005, "The effect of hydrogen addition on flammability limit and NOx emission in ultra-lean counterflow CH4/air premixed flames". Proceedings of the combustion institute, 30(1): p. 303-311.

[12] Hawkes, E.R. and J.H. Chen, 2004, "Direct numerical simulation of hydrogen-enriched lean premixed methane–air flames". Combustion and Flame, 138(3): p. 242-258.

[13] Jackson, G.S., et al., 2003, "Influence of H2 on the response of lean premixed CH4 flames to high strained flows". Combustion and Flame, 132(3): p. 503-511.

[14] K.K. Kuo, P.o.c., New York: John Wiley & Sons; 1986, p. 430.

[15] Kang, T. and D.C. Kyritsis, 2007" ,A combined experimental/computational investigation of stratified combustion in methane–air mixtures". Energy Conversion and Management, 48(11): p. 2769-2774.

[16] Leibovich, S., 1984, "Vortex stability and breakdown-Survey and extension". AIAA journal , :(9)22p. 1192-1206.

[17] Lipatnikov, A., Fundamentals of premixed turbulent combustion. 2019: CRC Press.

[18] Lipatnikov, A.N., 2017, "Stratified turbulent flames: Recent advances in understanding the influence of mixture inhomogeneities on premixed combustion and modeling challenges". Progress in Energy and Combustion Science, 62: p. 87-132.

[19] Lucca-Negro, O. and T. O'doherty, 2001, "Vortex breakdown: a review". Progress in energy and combustion science, 27(4): p. 431-481.

[20] Mardani, A., S. Tabejamaat, and M. Ghamari, 2010, "Numerical study of influence of molecular diffusion in the Mild combustion regime". Combustion Theory and Modelling, 14(5): p. 747-774.

[21] Nam, J. and J.J. Yoh, 2020, "A numerical investigation of the effects of hydrogen addition on combustion instability inside a partially-premixed swirl combustor". Applied Thermal Engineering, 176: p. 115478.

[22] Sahebjamei, M., E. Amani, and M. Nobari, 2019, "Numerical analysis of radial and angular stratification in turbulent swirling flames". Energy, 173: p. 523-539.

[23] Salavati-Zadeh, A., et al., 2018, "Kinetic simulation of flameless burners with methane/hydrogen blended fuel: Effects of molecular diffusion and Schmidt number". International Journal of Hydrogen Energy, 43(11): p.5983-5972 .

[24] Schneider, S., et al., 2019, "Structure of a stratified CH4 flame with H2 addition". Proceedings of the Combustion Institute, 37(2): p. 2307-2315.

[25] Sweeney, M.S., et al., 2012, "The structure of turbulent stratified and premixed methane/air flames II: Swirling flows". Combustion and Flame, 159(9): p. 2912-2929.

[26] Valorani, M., et al., 2006, "An automatic procedure for the simplification of chemical kinetic mechanisms based on CSP". Combustion and Flame, 146(1-2): p. 29-51.

[27] Wang, F., et al., 2015, "Routes of formation and destruction of nitrogen oxides in CH4/H2 jet flames in a hot coflow". International Journal of Hydrogen Energy, 40(18): p. 6228-6242.

[28] Wen, X., et al., 2021, "Flame structure analysis of turbulent premixed/stratified flames with H2 addition considering differential diffusion and stretch effects". Proceedings of the Combustion Institute, 38(2): p. 2993-3001.

[29] Zhou, R., et al., 2013, "Flow field measurements of a series of turbulent premixed and stratified

methane/air flames". Combustion and Flame, 160(10): p. 2017-2028.