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A NUMERICAL STUDY ON THE REDUCTION OF GREENHOUSE GASEOUS COMPONENT (CO_2) DUE TO THE ADDITION OF H_2 IN THE FUEL STREAM OF THE COUNTERFLOW CH_4/AIR DIFFUSION FLAME

Akter Hossain

[1]Department of Mathematical and Physical Sciences, East West
University, Jahurul Islam City, Aftab Nagar, Dhaka-1212, Bangladesh

akter.hossain@ewubd.edu and aakterh@yahoo.com

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Abstract

In this study, a series of 1-D and steady-state numerical simulations have been performed for the prediction of the effect of the addition of H_2 *on the characteristics of a non-sooting counterflow* CH_4*/Air diffusion flame using detailed chemical reaction model, which is composed of 325 elementary chemical reactions and 53 chemical species. Under the steady-state assumption, a set of one-dimensional transport equations of mass, momentum, species, and energy along with the equation of state has been solved numerically at the atmospheric conditions over the counterflow configuration by exploiting an efficient numerical code, OPPDIF (a Fortran Program for Computing Opposed-Flow Diffusion Flames). The grid adaption technique has been used to achieve better convergence as well as to ensure the maximum accuracy of the simulated results. It is found that the flame temperature is increased due to the addition of* H_2 *with* CH_4*, which is injected into the fuel stream. The elevation in the temperature is caused by the augmentation of the integrated heat release rate of the elementary reactions supported by the active radicals (H, O, and OH), which are generated by the higher reactivity of* H_2*. Besides, it is found that the mole fractions of* H_2O *are increased as the percentage of* H_2 *in the loading fuel (*CH_4*) is increased and also, it is identified that the chain propagating reaction,* $OH + H_2 \Rightarrow H_2O + H$ *is dominating one which produces highest amount of* H_2O*. Furthermore, it is noticed that the indirect greenhouse gas or precursor, CO is reduced when* H_2 *is added to* CH_4*. Consequently, the mole fraction of the principle greenhouse gas,* CO_2 *is decreased significantly when the fuel,* CH_4 *percentage is modified by the higher percentage of* H_2*. The sensitivity analysis of elementary* *reactions reveals the fact that the chemical reaction: OH + CO => H + CO_2 is a dominating reaction in producing a lower amount of CO_2 when the volume fraction of H_2 is increased in the fuel (CH_4) stream. In the presence of 75 % H_2 in CH_4, the pressure-dependent reaction, O + CO (+M) => CO_2 (+M) appears as another chemical route that also generates greenhouse gas, CO_2 but its contribution is negligibly small.*

Keywords: Numerical simulation, Methane, Counterflow diffusion flame, Green fuel (H_2), and Greenhouse gas (CO_2).

I. Introduction

The counterflow geometry is a fundamental geometrical configuration that is used to investigate the laminar diffusion flame physics where the fuel and oxidizer are flowing to each other from two opposite directions as shown in Fig.1 [V]. This geometry is very simple but important and very convenient for the theoretical development of diffusion flame physics, and hence the counterflow configuration has widely been used as a potential geometry [IX, X, XIII, XII, II, XI] until today in the experimental as well as in the numerical investigations for the elucidation of the flame physics as it represents purely one-dimensional laminar diffusion. Consequently, plenty of useful information about the basic properties of non-premixed (diffusion) combustion characteristics including the thermal and chemical structures of the flames can be understood very easily from the counterflow diffusion flames, especially under the laminar flow condition. Moreover, the counterflow geometry is relatively easy for the clarification of the fundamental flame parameters along with the underlying physical processes of the diffusion flames by employing minimum computational resources as the 1-D flame is generated regardless of the type of *fuels* under the counterflow configuration. One of the most widely used hydrocarbon fuels with lower carbon content is *natural* gas (also called *fossil* gas or *nonrenewable* gas) is a combustible gaseous hydrocarbon mixture consisting of methane as a primary chemical component in addition to various types of smaller amounts of other higher alkanes (e.g., $C_n H_{2n+2}$). The purest form of natural gas that has been delivered to our homes and industry, is almost pure methane. While burning CH_4 in the air, it produces carbon dioxide (CO_2) and water vapor (H_2O) as the major products along with heat and light. However, it is well-known that one of the principal greenhouse gaseous components is carbon dioxide (CO_2). Global warming is an environmental issue that is closely related to global weather and climate change owing to the increment in the level of the ‘greenhouse gaseous’ component in the atmosphere. There are certain gases in our atmosphere that control the amount of heat generation which is available in the neighborhood of the earth's surface. Based on this fact, scientists and researchers have hypothesized that an increase in these greenhouse gases transforms into an increase in the local temperature field around the globe, which gives rise to an alarming adverse environmental effect [XX]. Consequently, one can say easily that it would be quite difficult for the survival of lives on this earth in the near future, if no treatment has been made regarding this matter as mentioned above. To control the emission of greenhouse gases (i.e., the paramount chemical component, CO_2), it is indispensable to reduce the usage of burning natural gas (CH_4) in practical combustion devices such as various types of engine systems for the production of thermal energy from the chemical energy. Subsequently, this thermal energy is then converted to mechanical energy and electrical energy which mitigate the major energy demands for our modern society. So, a question naturally may arise in our potential readers' minds on how to supply the necessary energy demand without producing or reducing the percentage of greenhouse gases like carbon dioxide (CO_2). One of the potential solution techniques would be the complete replacement or partial replacement of natural gas (CH_4) by green fuels such as hydrogen (H_2) during the production of energy as required to make our life comfortable, sustainable, and free from global warming-related severe environmental impacts. *These dire environmental events have motivated us to conduct this piece of research work.* Consequently, we have devoted ourselves to finding alternative sources of hydrocarbon fuels or partial replacement of hydrocarbon fuels by the gaseous chemical compound which does not contain any carbon atom. With this in our mind, we have made an extensive review of the open literature on the addition of the carbon-neutral chemical molecule, H_2 with hydrocarbon fuels that burn in the presence of an oxidizing agent over the counterflow geometrical configuration (see Fig. 1) for producing the counterflow diffusion flames [III, VI, VIII, I, XIV, XVI]. These enormous research works have been carried out by legendary researchers and scientists under different pertinent conditions as appropriate while the addition of H_2 in different proportions with the targeted fuel is treated as one of the numerical as well as experimental parameters, and they have pointed out that both thermal and chemical structures of the counterflow diffusion flames have modified significantly along with the soot formation mechanism, its growth characteristics and the pollutant emissions and so on. Unfortunately, the concrete, straightforward, and systematic research findings along with the future guidelines have *not* been reported by the authors as cited above regarding the reduction strategies for the precursor, CO of greenhouse gas and the principal greenhouse gaseous component, CO_2 when the enrichment of H_2 in the fuel stream has been made in their studies. Consequently, one can easily conclude that the aforementioned studies have left *a* '*research gap/space*' for the researchers/scientists in conducting further research works on the subject of H_2 addition systematically with the hydrocarbon fuels to fill the '*researcher gap*' as left by the researchers adopting appropriate strategies to reduce the concentration of precursor (CO) of the principle greenhouse gaseous component (CO_2). Thus, we have taken this issue as described above as our main research target in this work. To reveal the fact as expected, we have to find a stable source for the production of a carbon-neutral chemical component, H_2. It is well-known that around 95% of hydrogen (H_2) has been produced by employing the traditional thermochemical method in cooperation with the hydrocarbon route due to its lower production costs. Since each technique has its pros and cons, one of the demerits of this process is the generation of carbon and its associated chemical compounds, especially when no *carbon-captured device* has been installed in the system. However, one of the eco-friendly and commercially available alternative technologies by which we can produce huge amounts of hydrogen (H_2) as required is known as *electrolysis.* It is worthy to mention here for the potential readers' convenience that the *electrolysis* is required to be defined in a very simplified way. *Electrolysis* of water (H_2O) is the technique in which electricity has been used directly to split water (H_2O) into oxygen (O_2) and hydrogen gas (H_2). Hydrogen (H_2) gas which is generated in this technique can be used as a future clean fuel. Besides, by remixing this H_2 with the oxygen (O_2), the combustible *oxyhydrogen gaseous* mixture can be generated, which can be burned to obtain clean energy as well. However, from an economical point of view, an *electrolysis* process is a costly process as compared to the former process and therefore, the hydrogen (H_2) which is produced through electrolysis technology using water (H_2O) as a renewable energy source is called 'green hydrogen' [XVIII]. Hence, in this study, the thermal and chemical structures of the counterflow diffusion flame will be analyzed by adding 'green hydrogen' in the fuel stream when nothing has been added externally in the oxidizer i.e., Air (N_2: 79% + O_2: 21 %) stream. It means that in the oxidizer stream, air is allowed to enter into the system which contains O_2: 21 %, and thus a CH4/Air counterflow diffusion flame can be established over the counterflow configuration (see Fig. 1). Therefore, we expect that a unique feature of CH_4/Air counterflow diffusion flame, in terms of thermal and chemical structure including the precursor (CO) of greenhouse gas and the principle greenhouse gaseous component (CO_2) will be revealed through this study when the fuel stream (CH_4) has been modified by the various mole fraction of green, H_2. Consequently, our main target which is described above will be fulfilled as expected.

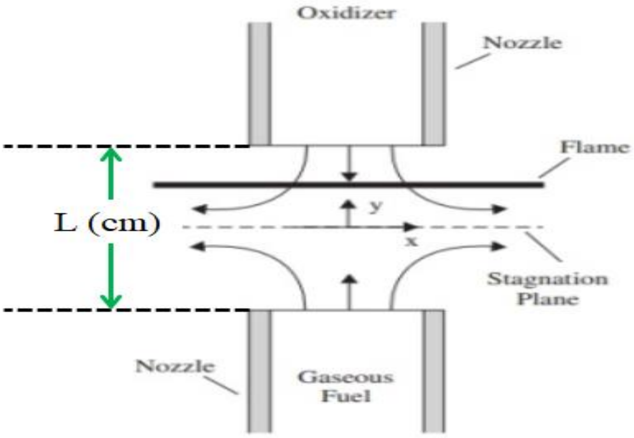

Fig. 1. Schematic setup for the counterflow geometry in producing 1-D flat counterflow diffusion flames [V] where fuel and oxidizer are injected into each other from opposite directions.

Since the counterflow CH_4/Air diffusion flame under current conditions provides *purely 1-D laminar diffusion flame* [IV] along with *an* extensive and detailed chemical reaction mechanism for highly reactive CH_4-Air mixtures in the presence of H_2 at fuel stream, the findings of this study especially the purely 1-D laminar flat flame along with its properties (i.e., chemical and thermal structure) can be treated as the potential building block for the development of an efficient mathematical model for turbulent combustion, which generally occurs in the practical combustors such as automotive engines, aero-engines, jet engines, turbo-engine, gas turbine engines and so on.

II. Methodology: Computational approaches

The counterflow CH_4/Air diffusion flame configuration is considered to be vitally important configuration which has two opposing ports for fuel and oxidizer apart from L= 2 cm as shown in Fig. 1. Both fuel (CH_4) and air (79% N_2 + 21 % O_2) are injected into the system of interest (see Fig. 1) at a fixed velocity of 25 cm/s with temperature of 300 K under normal atmospheric condition (i.e., pressure = 1 atm). It should be mentioned here that the volume fraction of methane (CH_4) has been modified by adding the different volume fractions of pure hydrogen (H_2) in the fuel stream to capture the influence of H_2 addition on the counterflow diffusion flame structures and its influence in the reduction of the generation of greenhouse gaseous component (CO_2). The variation of fuel by adding H_2 to the fuel stream has been made in this study and it is treated as a *numerical parameter* only in this study. Besides, the mixture-averaged diffusion model based on Fick's law is applied in this study to handle the molecular diffusion of various chemical species. Besides, the detailed chemical reaction mechanism [XVII] involving 325 elementary chemical reactions associated with 53 chemical species has been used to carry out this simulation. The total number of grid points of 250 has been considered over the distance L = 2 cm. In addition, the grid adaption technique has been imposed in this study for better convergence and to perfectly resolve the thermal and chemical structures of the flame. We have also specified the maximum number of grid points, 10 that will be added at a time during the grid adaptation process. This adaptation technique has been found to yield significant improvements in the accuracy of numerical results against the fixed-grid method.

To discretize the *governing equations*, we have used the upwind scheme to ensure smooth numerical convergence along with stability by controlling the boundedness of the solutions as it has diffusive characteristics. Although the upwind scheme tends to drop some physics to some extent, the dominating phenomena have been well captured as found in our earlier work [IV]. This dropping event as mentioned above has been indemnified by applying a robust and dynamic grid point adaptation technique during the calculation to resolve all tiny physical and chemical aspects that are related to the counterflow CH_4/Air diffusion flame physics.

It is known to all those who are engaged in research in the fields of combustion science and engineering or chemical engineering that any combustible mixture will not start burning automatically. An external heat source is necessary to ignite the combustible mixture. In this study, a temperature profile is constructed numerically by imposing the temperature of 300 K at L= 0 cm and L = 2 cm, and the temperature of 2400 K at L = 0.25 cm to L = 1.5 cm, which looks like very similar to the shape of an isosceles trapezoid. Hence, this temperature profile has been used as an initial guess profile to ignite the combustible mixture successfully in the present study. It should be noted here that this profile has been found to work successfully in igniting the combustible mixture in a series of numerical studies in the field of combustion research, for instance, [IV].

Besides, it is worth mentioning here that the same set of governing 1-D steady-state transport equations is applied in the present calculation as we have used in our earlier study, which has mainly focused on the development of the relation between the flame chemiluminescence and the heat release rate (HHR), accomplished by *Hossain and Yuji* [IV]. For the sake of brevity, the governing equations have not been presented here but the potential readers will find the information of these fundamental set of transport equations for counterflow diffusion flame very easily elsewhere in the open literature of combustion research, for instance in ref. [IV]. However, a set of one-dimensional steady-state transport equations of mass, momentum, species, energy along with the equation of *state* has been solved numerically under the pertinent conditions by Fortran code (OPPDIF) [VII] over the counterflow configuration (Fig.1). In this study, the modification of CH_4 in the fuel stream is made by adding the different mole fraction of H_2 and this kind of blending effect is expected to be revealed a unique feature for the counterflow CH_4/Air diffusion flame as expected that is the reduction of greenhouse gaseous component (CO_2), which is the goal of our study.

III. Results and discussion

III.i Chemical and thermal structures of counterflow CH4/Air diffusion flame

Figure 2 represents the chemical structures or the consumption pattern of CH_4 and O_2 for the counterflow CH4/Air diffusion flame when H_2 is added to the fuel stream. At first, it should be clarified whether the applied conditions in terms of blending effects (i.e., H_2 addition in the fuel stream) are perfectly reflected in the distribution of the mole fractions of CH_4 which are captured numerically over the distance L = 2 cm (see Fig. 1). It is apparent in this figure that the **red colored solid-line** which has been used to represent the numerically

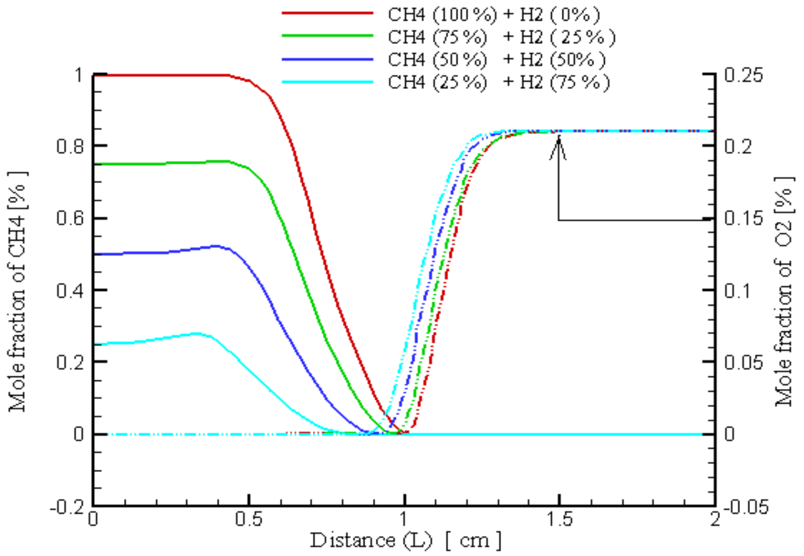

Fig. 2. The chemical structures (represented by the mole fraction of CH_4 and O_2) of counterflow CH4/Air diffusion flame over the distance (L = 2 cm) (see Fig 1) for the addition of different mole fractions of H_2 in the fuel stream.

obtained mole fraction of CH_4 when the pure 'CH_4 (100 %) + H_2 (0 %)' is injected into the system of interest through the fuel stream. Consequently, the *numerical* *finding* after the execution of **OPPDIF** for the aforesaid condition embedded in Fig. 2 agrees well with that of the imposed numerical condition for the mole fraction of fuel at fuel stream (L = 0.0 cm). This agreement explicitly tells us the mole fraction of CH_4 remains unchanged (i.e., pure CH_4: 100%) which has been supplied at L = 0.0 cm (see red colored solid-line). Furthermore, one can easily observe in this figure that due to the addition of H_2 with CH_4 at L = 0 cm (fuel stream), the mole fraction distribution is decreased over L for all of the conditions considered in this study. Apart from this, in the counterflow configuration, the mole fraction of fuel (CH_4) and air is injected into the system from two opposing nozzles having the same velocity of 25 cm/s located apart from each other at a distance, L = 2 cm. Hence, the fuel and air are mixed instantaneously by molecular diffusion which gives rise to a stagnation plane between two opposing nozzles, and consequently, a stoichiometric mixing line is generated in the vicinity of the stagnation plane. Once this mixing line experienced the existence of the initial temperature profile as described in the preceding section, the oxidation processes between fuel (CH_4) and air are started immediately. As a result, the consumption/reduction in the mole fraction of CH_4 and O_2 occurs gradually around the middle point over the distance, L = 2 cm, and eventually, the mole fraction of CH_4 and O_2 becomes zero for all cases as presented in Fig. 2 at the vicinity of L = 1 cm by giving rise to a nearly **V-shaped cavity** over the zone of $0.5 \text{ (cm)} \leq L \leq 1.25$ (cm). This is the most common fundamental features (that are well-known to all in the field combustion research regime) of the counterflow diffusion flame which are captured by the present numerical simulation. Since this fundamental characteristic of the counterflow diffusion flame has been captured by the present numerical simulation, it proves that our numerical simulation is reasonably accurate in producing the counterflow diffusion flames. Additionally, this event can be treated here as an indirect validation of our numerical calculation, although no specific data of the experimental investigation for the counterflow diffusion flame has been compared with that of the present numerical data. Further inspection of Fig.2, it reveals a very interesting fact that the above-mentioned **V-shaped cavity,** over the zone of $0.5 \text{ (cm)} \leq L \leq 1.25$ (cm) formed by the structures of the consumption of mole fraction of CH_4 and O_2, is narrow when pure CH_4 is injected into the system from the fuel stream. In contrast, the V**-shaped cavity** becomes wider as H_2 is added in different volume fractions with CH_4 due to the fact of high diffusive properties of H_2. The law of mass conservation in physical chemistry states that the mass of the reactants must equal to mass of the products. This law is valid in any combustion system accompanied by the generation of heat and light in the form of flames of different kinds such as premixed, non-premixed (diffusion), partially premixed, laminar, and turbulent. Since it is found in Fig. 2 that both reactants CH_4 and O_2 are consumed by giving rise to a V**-shaped cavity**, according to mass conservation law, one can easily infer that the present counterflow reacting system will have the production records of the rest of the species as presented in Table: 1 in conjunction with the temperature which is the measure of the intensity of the total heat generated by all chemical reactions involved in the applied chemical reaction mechanism to carry out present numerical simulation.

Figure 3 shows the thermal structures (represented by temperature field) of the counterflow CH_4/Air diffusion flame due to the addition of different mole fractions of H_2 with CH_4, captured over the distance *(L* = 2 cm) as shown in Fig. 1. It is clear in Fig. 2 for the condition of ‘CH_4 (100 %) + H_2 (0 %)’, that the maximum flame temperature is located around 1 cm over the distance (*L*) where the mole fractions of CH_4 and O_2 are found to be consumed i.e., the V-shaped cavity is generated as presented in Fig. 2. Besides, it is also noticed that the maximum temperature is increased due to the increment in the mole fraction of H_2 which is added with fuel at the fuel stream. Although the pictorial representations for the enhancement of the mole fractions of O, H, OH, and H_2 due to the blending of CH_4 with H_2 have not been shown here for the documental brevity, however, the authors have confirmed it. So, it is worthy to mention here for the convenience of potential readers’ that the above-

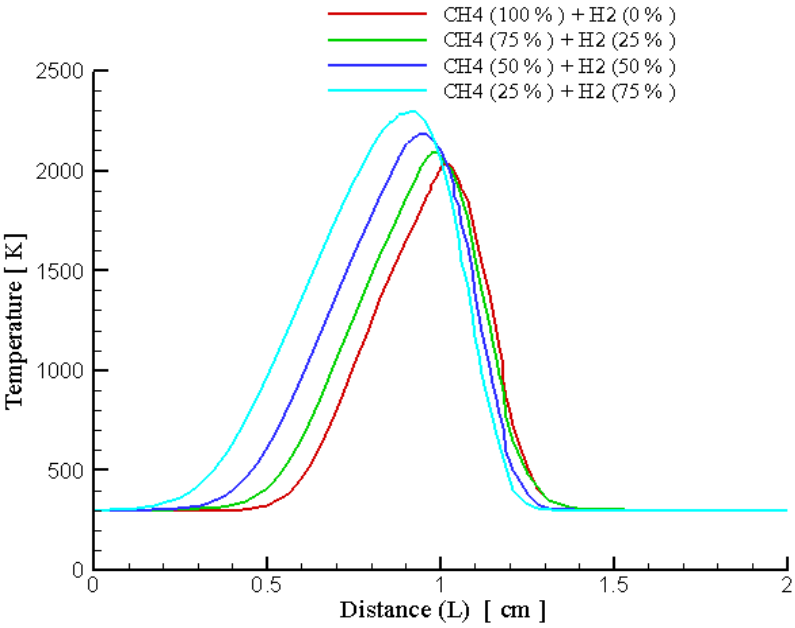

Fig. 3. The thermal structures (represented by temperature) of counterflow CH_4/Air diffusion flame over the distance (L = 2 cm) (see Fig. 1) for the addition of different mole fractions of H_2 in the fuel stream.

stated chemical components are increased when H_2 is added to CH_4. Thus, the scenario of the increment of temperature is supposed to happen owing to the promotion of the generation of the active radical pool in H_2 chemistry such as O, H, and OH, and the stable molecules like H_2 and O_2 (see Fig. 2) as well. Consequently, the elementary reaction paths that are dominated by this radical pool as well as the stable molecules give rise to an increase in the total heat release rate in the counterflow reacting system, and thus the local temperature is supposed to be increased in this system. These observations such as an increment in the temperature and an enhancement of the generation of the radical pool composed of O, H, and OH *agreed qualitatively* with the earlier study on the premixed flame accomplished by V. K. Yadav et. al. [XV] under the H_2 enrichment condition with biogas. To wipe out the potential readers' confusion, it should be mentioned here the fundamental flame physics is independent of the modes [i.e., premixed and non-premixed (diffusion flame)] of the flames. Thus,

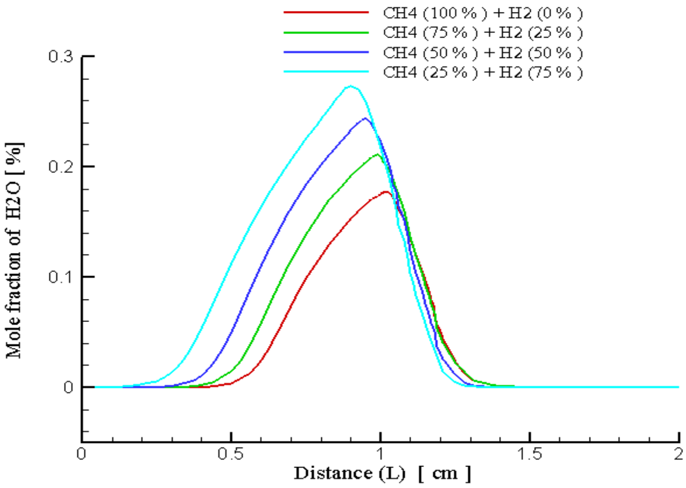

Fig. 4. The chemical structure (represented by the production of the mole fraction of H_2O) of counterflow CH4/Air diffusion flame over the distance (*L* = 2 cm) (see Fig. 1) for the addition of different mole fractions of H_2 in the fuel stream.

one can easily conclude that these evidences are the passive validation of the present numerical model and the corresponding findings as well. In the next paragraphs, we are going to illustrate vitally important and major chemical products of the present counterflow CH_4/Air combustion system.

Figure 4 represents one of the major and final products of CH_4/Air counterflow diffusion flame which is the mole fractions of H_2O. It is pretty clear to anyone that the mole fraction of H_2O is increased as the addition of H_2 with CH_4 has been increased in a manner as shown in the legends of this figure. This increment in the production of the combustion process is due to fact of an enhancement in the generation of the radical pool involving O, H, and OH, and accordingly, the reaction paths (i.e., $OH + H_2 \Rightarrow H_2O + H$, $H + OH + M \Rightarrow H_2O + M$, $OH + HO_2 \Rightarrow O_2 + H_2O$, $OH + H_2O_2 \Rightarrow HO_2 + H_2O$) which are responsible for the generation of H_2O. It is noticed from these elementary paths that the hydroxyl radical, OH belongs to the radical pool which has highly reactive characteristics and thus it is participating in all of the reactions as presented above. Further inspections of the above reactions are made by adopting sensitivity of analysis, it has been confirmed that the chain propagating reaction, $OH + H_2 \Rightarrow H_2O + H$ is the dominating one which produces the highest amount of H_2O in the present reacting system. However, before going to examine another indispensable product, CO_2 for this counterflow CH_4/Air diffusion flames, we would like to examine the characteristics of the mole fraction CO which is identified as an important indirect greenhouse gas [XX] or the precursor of the ultimate/ principle greenhouse gas, CO_2 in CH_4/air combustion system.

Figure 5 depicts the mole fraction distribution of a precursor of greenhouse gas, CO when the loading fuel at the fuel stream is modified by the different mole fraction of H_2 in the counterflow configuration as represented in Fig. 1. It is very apparent that the potential reader’s even who are not an expert of *combustion chemistry* can easily conclude from Fig. 5 that the mole fraction CO is decreased as the mole fraction H_2 addition in CH_4 is increased at

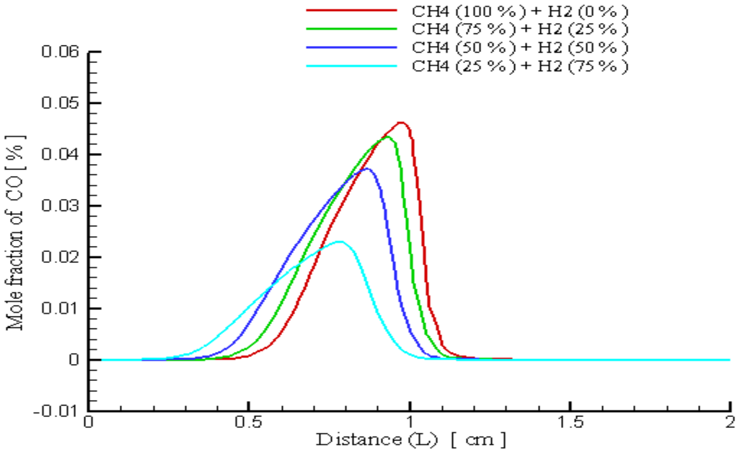

Fig. 5. The chemical structure of the precursor of greenhouse gas (represented by the mole fraction of CO) of counterflow CH_4/Air diffusion flame over the distance ($L = 2$ cm) (see Fig. 1) for the addition of different mole fractions of H_2 in the fuel stream.

fuel stream. Besides, it is clear in Fig. 5 that the apical value of the mole fraction distribution of CO under the condition of pure CH_4 is reduced drastically around 50% when 75% H_2 has been added to CH_4, and the location of apical values of CO over L = 2 cm for different the conditions as found in the legend is shifted towards the fuel stream when the mole fraction CH_4 is modified by H_2 (0% to 75%). This event happened due to the fact of shifting in the distribution of the mole fraction of O_2 towards the fuel stream as presented in Fig. 2. The physical reason behind the scenario as pointed out above would be the lightest molecular weight of H_2 which eventually contributes to the higher diffusive behavior of H_2 towards the fuel side for which the promotion of the oxidative chemical routes of H_2 occurs towards the fuel side by which the active radical pool, as mentioned in the preceding section, is generated accordingly towards the fuel side. Consequently, one would see the same tendency in the case of the principle combustion production in the CH_4/Air combustion process that is H_2O in the present reactive system. Since the precursor of greenhouse gas (CO) is decreased due to the addition of H_2 in CH_4, one can expect that the production of principal greenhouse gas (CO_2) would decrease to some extent accordingly.

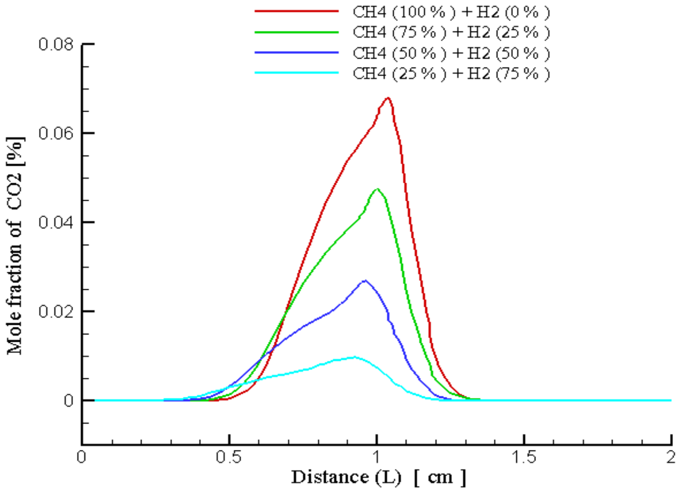

Fig. 6. The chemical production structure (represented by the mole fraction of principle greenhouse gas, CO_2) of counterflow CH4/Air diffusion flame over the distance (L = 2 cm) (see Fig. 1) for the addition of different mole fractions of H_2 in the fuel stream.

Figure 6 shows the distribution of the mole fraction of the principal greenhouse gas, CO_2 when the various percentage of the mole fraction of carbon-neutral chemical compound, H_2 has been as described in the legend of this figure. It is very much clear to anyone that the mole fraction of the principal greenhouse gaseous component, CO_2

is found to be reduced as the mole fraction of H_2 is increased. This decrement in the mole fraction of CO_2 is due to the fact of the precursor chemical component, CO as present in Fig. 5. Although the sensitivity of analysis of the result has not been performed extensively for all results represented here for the documental brevity, however, the dominating reaction route that is responsible for lowering the concentration of the principle greenhouse gaseous compound, CO_2 has been detected by the rigorous sensitivity analysis of the chemical reactions which is presented for two cases: (a) CH_4 (100%) + H_2 (0%) and (b) CH_4 (25%) + H_2 (75%) as shown in Fig.7. In figure 7, it is clear that the dominating chemical route is OH + CO => H + CO_2 for the production of ultimate greenhouse gaseous component, CO_2 for cases as illustrated in Fig. 7. Further scrutiny of Fig. 7, it unveils the fact that the mole fraction, CO_2 is reduced by one order for case (b) as compared to case (a). Besides, it is also clear in Fig. 7 that the imposition of condition (b) leads to a slight promotion of another chemical reactive channel which is influenced by the pressure of the system, and it gives rise to a little amount of greenhouse gas (CO_2) leaving the reaction: OH + CO => H + CO_2 as an influential chemical route among the reactions for the production of the principle greenhouse gas, CO_2. However, a slight increment in the production of CO_2 by the pressure-dependent reaction: O + CO (+M) => CO_2 (+M) and HO_2 + CO=> OH + CO_2 are observed in Fig. 7 (b) and both of which have negligible role in the production of CO_2 where M is the concentration of the combustible mixture, possibly including enhanced third-body efficiencies.

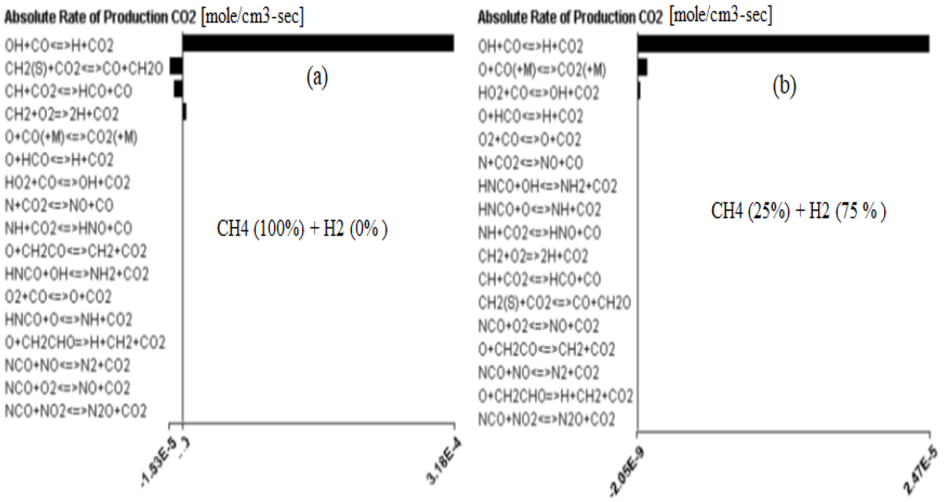

Fig. 7. The sensitivity of analysis for detecting the main route of chemical reaction that produces principal greenhouse gas, CO_2 in counterflow CH_4/Air diffusion flame over the distance (L = 2 cm) (see Fig. 1) for the addition of different mole fractions of H_2 in the fuel stream where (a) CH_4 (100 %) + H_2 (0%) and (b) CH_4 (25%) + H_2 (75%)

IV. Conclusions

In this investigation, 1-D, steady-state, non-sooting counterflow CH_4/Air diffusion flames have been simulated using an efficient Fortran numerical code (OPPDIF) to examine the behavior of thermal (temperature) and chemical structure (mole fraction of CH_4, O_2, H_2O, CO, and CO_2) of the CH_4/Air counterflow diffusion flame when hydrocarbon fuel CH_4 is blended by the various percentage of H_2 at the fuel stream. The modification of pure CH_4 by the different proportions of H_2 has been treated in this numerical study as the only one *numerical parameter* and the injecting velocity of 25 cm/sec has been kept constant at both fuel and air streams throughout this study. Detailed combustion chemistry has been applied in this study which includes 325 chemical reaction steps and 53 chemical species. The mesh adaptation technique has been applied to resolve the thermal and chemical structures to obtain better accurate numerical results thereby elucidating that our main target of this study is to reduce the greenhouse gaseous chemical component during the combustion process which flame is stabilized over the counterflow configuration. However, from the present 1-D, steady-state numerical study, we can synopsize our key findings as follows:

1. The local maximum flame temperature is found to be increased due to the addition of the mole fraction H_2 with CH_4 at the fuel stream. The increment in the temperature is observed due to the fact of the generation of the active radical pools in a counterflow reactive system such as O, H, and OH, and the stable molecules such as H_2 and O_2 as well. Consequently, the elementary reactions which are influenced by the aforesaid radicals as well as stable molecules are enhanced, which gives rise to an increment in the total heat release rate of reactions involved in the adopted chemical reaction scheme and as a result, the local temperature is found to be increased in the system.

2. One of the major and final products of the CH_4/Air counterflow diffusion flame system is the mole fractions of H_2O. It is apparent to everybody that the mole fraction of H_2O is increased when the percentage of H_2 in CH_4 has been increased at the fuel stream. The increment in the production rate (mol/m^3.sec) is due to the fact promotion of the reaction, $OH + H_2 => H_2O + H$ as the concentration of active radical OH is enhanced by the addition of H_2 with CH_4 at the fuel stream.

3. The mole fraction distribution of the dominating precursor of the greenhouse gas, CO is decreased when the loading fuel is modified by the different mole fraction of H_2 under counterflow geometrical configuration. It is very apparent that the potential reader even those who are not an expert in *combustion chemistry* can

easily conclude from Fig. 5 that the mole fraction CO is decreased as the mole fraction H_2 addition in CH_4 is increased at the fuel stream.

4. The ultimate goal of this research is to reduce the mole fraction or concentration of the principal greenhouse gas, CO_2 in a counterflow system which has been well-captured in our current system that the mole fraction of CO_2 is decreased significantly when the loading fuel is modified by the higher percentage of H_2 under counterflow configuration. The sensitivity analysis finally reveals the fact that the chemical reaction: $OH + CO => H + CO_2$ appears to be a dominating reaction for the production of $CO_{2,}$ once the precursor or indirect greenhouse gas, CO is generated in the reacting system. However, it is also found that the pressure-dependent reaction, $O + CO (+M) => CO_2 (+M)$ emerged as another reaction route for the production of the principal greenhouse gas, CO_2 when the mole fraction H_2 addition in CH_4 is increased significantly at the fuel stream. However, the contribution of the later reactive path has a negligible role in giving rise to CO_2.

Although the present study has been conducted under the constant strain rate (i.e., the gradient of velocity) at both streams of the counterflow geometry, the strain rate can be varied to capture much more quantitative insights into the chemical reactions for which the generation of principle greenhouse gas (CO_2) at atmosphere can be controlled. Besides, another potential candidate, syngas can also be added with CH_4 to detect the key chemical reaction path that is directly connected with the generation/consumption of CO_2 along with its precursor CO by interplaying the compositions of syngas elements i.e., CO and H_2. The research work as represented above, with the aim of extensive sensitivity analysis of elementary reaction paths for the identification of the production and consumption channel of chemical species, is now under progress, and hence the findings of the ongoing research are expected to be reported elsewhere soon.

Table: 1 Chemical Reaction Mechanism (detailed chemical reaction Scheme) [XVII] has been used in this study.

➢ Chemical elements: O H C N AR ➢ Total Number of chemical species: 53 H_2 H O O_2 OH H_2O HO_2 H_2O_2 C CH CH_2 $CH_2(S)$ CH_3 CH_4 CO CO_2 HCO CH_2O CH_2OH CH_3O CH_3OH C_2H C_2H_2 C_2H_3 C_2H_4 C_2H_5 C_2H_6 HCCO CH_2CO HCCOH N NH NH_2 NH_3 NNH NO NO_2 N_2O HNO CN HCN H_2CN HCNN HCNO HOCN HNCO NCO N_2 AR C_3H_7 C_3H_8 CH_2CHO CH_3CHO
➢ Total number of reactions: **351**

- The reaction rate is evaluated by Arrhenius law: $AT^b \exp(-E/RT)$ and the units of Arrhenius parameters are follows:

    I. Preexponential factor: **A**: cm3 /mol·s)
    II. Temperature exponent: **b** (unitless)
    III. Activation Energy: **E** (cal/mol)
    IV. Universal gas constant: **R** (1.87 cal/mol. K)
    V. Local temperature: **T** (K)

Reactions	**A**	**b**	**E**
R1. $2O+M<=>O_2+M$	1.200E+17	-1.000	0.00
H_2/ 2.40/ H_2O/15.40/ CH_4/ 2.00/ CO/ 1.75/ CO_2/ 3.60/ C_2H_6/ 3.00/ AR/ 0.83/			
R2. $O+H+M<=>OH+M$	5.000E+17	-1.000	0.00
H_2/2.00/ H_2O/6.00/ CH_4/2.00/ CO/1.50/ CO_2/2.00/ C_2H_6/3.00/ AR/ 0.70/			
R3. $O+H_2<=>H+OH$	3.870E+04	2.700	6260.00
R4. $O+HO_2<=>OH+O_2$	2.000E+13	.000	0 .00
R5. $O+H_2O_2<=>OH+HO_2$	9.630E+06	2.000	4000.00
R6. $O+CH<=>H+CO$	5.700E+13	0.000	0.00
R7. $O+CH_2<=>H+HCO$	8.000E+13	0.000	0.00
R8. $O+CH_2(S)<=>H_2+CO$	1.500E+13	0.000	0.00
R9. $O+CH_2(S)<=>H+HCO$	1.500E+13	0.000	0.00
R10. $O+CH_3<=>H+CH_2O$	5.060E+13	0.000	0.00
R11. $O+CH_4<=>OH+CH_3$	1.020E+09	1.500	8600.00
R12. $O+CO(+M) <=>CO_2(+M)$	1.800E+10	0.000	2385.00
LOW/ 6.020E+14 0.000 3000.00/ H_2/2.00/ O_2/6.00/ H_2O/6.00/ CH_4/2.00/ CO/1.50/ CO_2/3.50/ C_2H_6/3.00/ AR/ .50/			
R13. $O+HCO<=>OH+CO$	3.000E+13	0.000	0.00
R14. $O+HCO<=>H+CO_2$	3.000E+13	0.000	0.00
……………………………………………………………………………………… ***The reactions from R15 to R344 have not been shown here for the brevity of pages as the presentation of the whole reaction mechanism requires a couple of pages***……………………………………………………………………………			
R345. $O+C_3H_7<=>C_2H_5+CH_2O$	9.640E+13	0.000	0.00

R346. H+C_3H_7(+M) <=> C_3H_8(+M)	3.613E+13	0.000	0.00
LOW/ 4.420E+61 -13.545 11357.0/ TROE/0.315 369.0 3285.0 6667.0 / H_2/2.00/ H_2O/6.00/ CH_4/2.00/ CO/1.50/ CO_2/2.00/ C_2H_6/3.00/ AR/ 0.70/			
R347. H+C_3H_7<=>CH_3+C_2H_5	4.060E+06	2.190	890.00
R348. OH+C_3H_7<=>C_2H_5+CH_2OH	2.410E+13	0.000	0.00
R349. HO_2+C_3H_7<=>O_2+C_3H_8	2.550E+10	0.255	-943.00
R350. HO_2+C3H_7=>OH+C_2H_5+CH_2O	2.410E+13	0.000	0.00
R351. CH_3+C3H_7<=>2C_2H_5	1.927E+13	-0.320	0.00

Conflict of Interest:

The author declares that there was no conflict of interest regarding this paper.

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