Numerical Simulation Study on the Effects of Diatomic Gas Addition on Soot and Its Precursors in Acetylene Premixed Flame

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Abstract - In order to study the PAHs and soot volume fraction, CHEMKIN software was used for the analysis of H_2 , CO and N_2 effects on the PAHs and soot formation in a premixed laminar C_2H_2 flame numerically. To have good understanding on effects of additives on PAH formation and intermediate species like OH, H_2 and C_2H_2 , C_3H_3 , C_4H_4 , C_5H_5 and soot volume fraction, some simulations were performed under different addition ratios (0%, 20% and 40%) of H_2 , CO and N_2 . The ABF mechanism which includes C_1 and C_2 chemistry, PAH growth was used to understand the particle inception and mole fractions of intermediate species. Prior to performing simulation, the performance of model prediction for soot, PAH and mole fraction of intermediate products was validated and calculations were performed and compared with the experimental results. Hydrogen showed strong chemical effect when it is added into the unburned mixture. The mole fractions of important soot antecedent species such C_2H_2 and PAH were inhibited significantly as compared to the cases of CO/N₂ addition. However, the aromatic radical is limited by the excess of H_2 , thus causing the lower production rate of large PAHs. In addition, results showed that hydrogen, carbon Monoxide and nitrogen additions lead to the reduction of temperature. To study the effects of additions on soot generation, $N_2/CO/H_2$ were added to C_2H_2/air flame from 0% to 40%. The results showed that $N_2/CO/H_2$ reduced the soot volume fraction.

Keywords: H₂/CO/N₂ addition; Polycyclic Aromatic Hydrocarbon; Premixed Flame; Soot;

1. Introduction

At present, the world's vitality request is relying upon the ignition of non-renewable energy sources, while the burning of petroleum derivative produces NOx and CO₂ pollutants and hydrocarbons including polycyclic aromatic hydrocarbons (PAHs) compounds and different contamination unavoidably [1], [2]. Polycyclic aromatics hydrocarbons are organic compounds having carbon and hydrogen and are the precursors of soot. Soot is one of the most important emissions of fossil fuels after combustion. Although the whole process of PAH and soot formation has been known but the in-depth process of PAH and soot formation and oxidation is required to be further understood. The detailed mechanism is the theoretical basis to guide the reduction of PAH and soot generation, so the study of PAH and soot generation within the flame is still a hot topic in today's society. Guo et al. [3] examined the effects on soot production in C_2H_4/air diffusion flames by adding CO and chemically constraining impact was qualified to the reduce the amount hydrogen atoms in the surface growth area and higher absorption of molecular hydrogen in the lower flame region. Gulder et al. [4] in his work presented the effects of H_2 in the ethylene, propane and butane jet diffusion flames and detected some uncertainties in visible flame length and along the diameter of flame. It was concluded that when H_2 was added in reasonable amount, a lesser impact on temperature field was detected. Choudhary and Gollahalli [5] investigated the structure of flame and attributes of diffusion flames of hydrogenhydrocarbon fuel in co-flowing air stream. In their work, it was seen that the length of flame was increased as propane quantity was increased in the mixture of hydrogen-hydrocarbon. Henríquez et al. [6] experimentally analysed the impacts of oxygen index against the soot production in co flow laminar, propane diffusion flames. In his study, he concluded that as the oxygen index increases with soot growth along with oxidation rate, the maximum soot volume fraction showed incremental rate with overall peak soot volume. Considerable amount of work exists in literatures focusing the influence adding hydrogen on soot formation. Particularly, premixed benzene and kerosene flames, caused a low increase in yellow luminosity by the addition of hydrogen[7].

The first objective of this work was to validate the model accuracy. Simulations were done and compared with the experimental data. After the model validation, the second objective of this work was to study or analyse the effects of H_2 , CO and N_2 additives in C_2H_2/air flame and also analyse their effects on major species, aromatic formation and soot volume fraction. The last but not least objective was to use the model to numerically evaluate the formation of PAH and soot in Laminar Premixed Burner Flame by using CHEMKIN software to advance the understanding of PAH and soot formation mechanism.

2. Numerical Model and Kinetic Model for Soot

Simulations were made in two steps for the evolution of particle. In first step, the concentration of the gaseous species and evolution of moments of soot particle size distribution was made [8]. Used a detailed simulation of the size of soot distribution chemical reaction mechanism in the gas phase [9] and soot formation [10]. Secondary by using Monte Carlo stochastic approach, the soot size distribution can be calculated. To find gaseous species use PREMIX flame code which is a CHEMKIN package subroutine [11]. The procedures of soot particles construction were depicted based on the detailed kinetic soot model and the method of moments created by Frenklach and co-workers [9].

Governing Equations

Equation for the one dimensional propagation of flame can represented as following [10]: Continuity Equation:

Energy Equation:

$$M = \rho u A \tag{1}$$

$$\dot{\mathbf{M}} \frac{dT}{dx} - \frac{1}{c_p} \frac{d}{dx} \times \mathbf{A} \frac{dT}{dx} + \frac{\mathbf{A}}{c_p} \sum_{\mathbf{K}=1}^{\mathbf{K}} \rho \mathbf{Y}_k \mathbf{V}_k c_{pk} \frac{dT}{dx} + \frac{\mathbf{A}}{c_p} \sum_{\mathbf{K}=1}^{\mathbf{K}} \dot{w}_k h_k \mathbf{W}_k = 0$$
(2)

Species Equation:

$$\dot{\mathbf{M}} \frac{dT}{dx} - \frac{1}{c_p} \frac{d}{dx} \times \mathbf{A} \frac{dT}{dx} + \frac{\mathbf{A}}{c_p} \sum_{\mathbf{K}=1}^{\mathbf{K}} \rho \mathbf{Y}_k \mathbf{V}_k c_{pk} \frac{dT}{dx} + \frac{\mathbf{A}}{c_p} \sum_{\mathbf{K}=1}^{\mathbf{K}} \dot{w}_k h_k \mathbf{W}_k = 0$$
(3)

Where, (k = 1,...,K), x represents spatial coordinate, M represents mass flow rate, T is for temperature, Y_k is the mass fraction of kth species, p is pressure, ρ is mass density, u is the velocity of the fluid mixture, W_k is the molecular weight of kth species, λ is the mixture thermal conductivity, c_p is the constant-pressure, \dot{w}_k is the molar rate of production by the chemical reaction of kth species per unit volume, h_k is the specific enthalpy of kth species, V_k is the diffusion velocity of kth species, A is the cross-section area of stream tube.

For the modelling of soot production, a model known as discrete section is used. And the development includes the reaction of gaseous species upto PAH, from the gas to particle formation process combined to elementary mechanism. Particles dynamical model incorporates nucleation, coagulation, and condensation of PAHs onto the surface of soot particles and surface development i.e., the introduction of acetylene to radical sites on surface, and oxidation process caused by hydroxyl radical and molecular oxygen.

Soot inception

The inception of soot is described by coagulation of PAH molecules. Production process of primary soot particles are being represented as dimerization of two molecules of pyrene.

$$PAH_i + PAH_j \rightarrow Soot_{i+j}$$
 (4)

$$R(t) = \frac{1}{2} \beta N_{PAHS} N_{PAHS}$$
⁽⁵⁾

Where, R(t) is the nucleation rate, β is the collision kernel, N_{PAHs} is the molar concentration of PAHs. Soot coagulation

Smoluchowski's equation is describing the soot coagulation process which is follow as:

$$G(i) = \frac{1}{2} \sum_{j=1}^{i-1} \beta_{j,i-j} N_j N_{i-j} - \sum_{j=1}^{n_{max}} \beta_{i,j} N_i N_j$$
(6)

Where, $\beta_{i,j}$ is the coagulation frequency.

Soot surface reaction

The condensation of pyrene and acetylene addition through HACA mechanism includes the surface growth reaction of soot.

$$Soot_i + A_4 \rightarrow Soot_{i+16}$$

(7)

$$Soot_i + C_2 H_2 \rightarrow Soot_{i+2} \tag{8}$$

Molecular oxygen and OH radicals in the oxidation process of soot particles, are considered to react with two gaseous.

$$Soot_i + OH \rightarrow Soot_{i-1}$$
 (9)

$$Soot_i + O_2 \rightarrow Soot_{i-2} \tag{10}$$

2.1. Model Validation

For the sake to validate present work, calculations were made and comparison was done to the experimental data of previous studies which is obtained in Figure 1, Figure 2 [9], Figure 3 [12] and Figure 4 [12]. As Figure 1 illustrate a typical premixed laminar flame structure, which consists of unburned mixture region, the transport region, the reaction region and burned mixture region.



Fig. 1: Schematic of one-dimensional premixed flame configuration.

Figure 2 demonstrates the simulated mole fraction of different species and temperature with the experimental data of previous studies [9] by ABF mechanism. It is clearly seen that there is good agreement between experimental data of mole fractions of major products and temperature with respect to HAB and calculated data. In all Figures the symbols are showing the experimental data while lines are representing the simulated data.



Fig. 2: Comparison of calculated and experimental data of mole fractions profiles for major products in pure C2H2/air flames [9] by ABF mechanism.

Figure 3 demonstrates the simulated mole fraction of benzene and naphthalene with the experimental data of studies [12]. It is clearly seen that the calculated date agreed well with experimental data of mole fractions of benzene naphthalene with respect to HAB by using ABF mechanism.



Fig. 3: Comparison of calculated and experimental data [12] of PAH in pure C₂H₂/air flames by ABF mechanism.

Figure 4 demonstrates the calculation of soot volume fraction and experimental data of previous studies [12]. It can be clearly understood that the calculated date showed excellent agreement with the experimental data of soot volume fraction with respect to HAB.



Fig. 4: Comparison of calculated and experimental data [12] of soot volume fraction in pure C2H2/air flames.

2.2. Boundary Conditions

The following tables 1 and 2 represent the calculation conditions for the simulation of C₂H₂/air Flame.

Quantity	Range
Pressure	0.12 bar
Initial	298 K
Tennedan	
Temperature	
Equivalence	2.75

Table 1: Calculation conditions for C2H2/air Flame.

H_2 , CO, N_2	0%	20%	30%
(Volume)			
C_2H_2	0.188	0.176	0.165
O ₂	0.171	0.166	0.162
N_2	0.641	0.623	0.607
H_2	0	0.035	0.066
CO	0	0.035	0.066
N_2	0	0.035	0.066

Table 2: Calculation conditions for C2H2/air Flame.

3. Results and Discussion

PAH with the addition of H₂, CO, N₂:

The production of Benzene (A1) by the decomposition of fuel is measured as a vital intermediate to develop PAH. Since, the production of Benzene changes the rate-limiting point in the reaction order to enhance PAHs. Figure 5(a) A1 has been as a function of the HAB. For the C₂H₂/H₂/air flames, the addition of hydrogen suppresses the formation of A1 near the burner surface. Due to the addition of hydrogen, mole fraction of A1, became higher and increases as the HAB increases. It is increased because the reverse rate of the H abstraction reaction due to abundance of H_2 . Therefore, converting more phenyls (A1-) into A1 (benzene). Similarly, the increased H_2 concentration can control further growth of PAH. Furthermore, Figure 5(b) elucidates the mole fraction of A2 which increased with a slightly fluctuated curves. After achieving its maximum value when the H_2 addition was 0% and 20%, A2 gradually decreased because the increased H_2 concentration can control further growth of PAH. On the other hand, 40% H₂ addition was totally different from 0% and 20% hydrogen addition because it depicts, more H₂ can control PAH growth near the maximum peak. Additionally, Figure 5(c) illustrates the mole fraction of A3. The mole fraction of 20% H2 addition was higher than 0% H₂. Contrary to this when H₂ was 40% it showed fluctuation from very beginning till its maximum value. Overall Figure 5(c) shows the mole fraction of A3 increased till a specific value, after that it will decrease even with addition of H_2 . Finally, Figure 5(d) shows the mole fraction of A4 decreases by adding the hydrogen. More hydrogen additive is having stronger chemical effect on A4 formation. That's why in $C_2H_2/H_2/air$ flame, the mole fraction of A4 was found lower. The H-abstraction C₂H₂-addition (HACA) mechanism for PAH growth can explain this actions. According to HACA mechanism the first aromatic ring of benzene (A1) is important.



Fig. 5: Mole Fraction (a)A1, (b)A2, (c)A3, (d)A4 with HAB.

As due diluent effect of CO which cause lower in C_2H_2 concentration results lower the PAHs production rate (which explained in chemical effects) which cause increases in A1, A2 and A3 with increasing HAB but the mole fraction of decreased by the addition of CO due to its diluent nature as presented in Figure 6(a)(b)(c)(d). Firstly, it can be seen that variation tendency of A1 and A2 are all increased firstly and decreased. The mole fraction of A1 and A2 decreased in a way from 0.5 to 2cm of HAB by the addition of CO as shown in Figure 6(a) and Figure 6(b). As it is represented in figure 6(c)&(d), the change trend of A3 and A4 are all increased and until to a flat state. The reduction of A4 is happened because of dilution. So, the increased CO concentration can control further growth of PAH due to dilution effect as shown in Figure 6.



Fig. 6: Mole Fraction (a)A1, (b)A2, (c)A3, (d)A4 with HAB.

As N_2 is affecting on C_2H_2 due to diluent in nature, thus the lower in C_2H_2 concentration results lower the PAHs production rate (which is explained in chemical effects) which cause decrease in A1, A2 and A4 with increasing HAB but the mole fraction of A3 increased by the addition of N_2 as mentioned in Figure 7(a)(b)(c)(d), represents the mole fraction of A1, A2, A3 and A4 as a function of HAB. So, the increased N_2 concentration can control further growth of PAH due to dilution effect as shown in Figure 7.



Fig. 7: Mole Fraction (a)A1, (b)A2, (c)A3, (d)A4 with HAB.

Thermal Effect:

The additions of H₂, CO, N₂ into C₂H₂/air laminar premixed flame affects thermally and their additions in C₂H₂/air flame decrease the temperature. From figure 8, it is worth mentioning flame temperature as function of HAB. When there was 0% addition of H₂, CO and N₂ in C₂H₂/air, the maximum temperature was 1742 K. By increasing the concentration of H₂, CO and N₂ in C₂H₂/air, the temperature decreases and for 20% concentration of H₂, CO and N₂ it reduced to 1710 K, 1719 K and 1725 K, respectively. Similarly, for 40% concentration of H₂, CO and N₂, the temperature reduced to 1682 K, 1691 K and 1710 K respectively. This showed that these all additives have thermal effect. H₂ had more significant effect on temperature than CO and N₂ did.



Fig. 8: Mole Fraction (a)A1, (b)A2, (c)A3, (d)A4 with HAB.

Chemical Effect on major species:

The effect of additives due to the chemical has been discussed. In order to know how the chemical reactions, influence the PAH, some important gas phase species were simulated.

Figure 9 (a) representing the mole fractions of OH. Reduction in mole fraction of hydroxyl is due to chemical effect with H_2 additions. By adding H_2 the rate of forward reaction is accelerated and it consumes more OH radical which causes

lower the OH radical quantity. Same time, more H atoms are formed. Reaching their peak values, mole concentrations of hydroxyl reduces quickly, with HAB. The following reaction might take place:

$$H_2 + 0H \rightarrow H_2 0 + H \tag{11}$$

When different percentage of H_2 is added in mole fraction of H_2 , the concentration of H_2 obviously increased. It is clearly seen in Figure 9 (b) that as increased the percentage of H_2 , quantity of H_2 also increased due to chemical effect. The following reaction might take place:

$$H_2 + H_2 \rightarrow 2H_2 \tag{12}$$

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The C_2H_2 /air pyrolysis is through the following reactions:

$$C_2H_2 + 0 \rightarrow CO + CH_2 \tag{13}$$

$$C_2H_2 + 0 \to H + HCCO \tag{14}$$

$$C_2H_2 + H \to C_2H_3 \tag{15}$$

As the concentration of H_2 increases with the mole fraction to the C_2H_2/air flame, from equation 14 the reaction is inhibited while the reaction of 15 is promoted. Considering the competition between the two reactions, the concentration of C_2H_2 decreases as shown in Figure 9 (c). Figure 9 (d) describes mole fraction of C_3H_3 with increased HAB. On the whole, the concentration of C_3H_3 first increased and then decreased to a flat state with HAB. The mole fraction is maximum at 0% H_2 addition and it continuously decreased with the addition of H_2 due to chemical effect. As Figure 9 (d) explains, when the H₂ was 20% the mole fraction was less than 0% and when H₂ was 40%, it showed an obvious different behaviour with fluctuated increase. In Figure 9 (e) the relationship between mole fraction of C_4H_4 (with 0%, 20% and 40% H_2 additive) and HAB has shown. It can be seen that the concentration of C_4H_4 presents a non-monotonic change, and its change trend increases first and then decreases with the increase of HAB. When 0% H₂ additive is used, the peak value of mole fraction is the maximum whereas the peak value is smaller for 20% and 40% H₂ additive conditions respectively. It is interesting to notice that for 40% H_2 additive, the decline after the peak value is slower than the other two cases, and the value is greater than in the other two cases. Figure 9 (f) depicts the relationship between mole fraction of C_5H_5 (with 0%, 20% and 40% H_2 additive) and HAB. As can be seen from the figure, the concentration of C_5H_5 gradually increases to a flat state with the increase of HAB. The graph shows when there was no H₂ additives the mole fraction of C₅H₅ is minimum, whereas for 20% H_2 additive the value of mole fraction C_5H_5 is maximum and for 40% H_2 additive it decreased more significantly than 20% H₂ additive case does.



Fig. 9: Mole Fractions of a) OH, b) H₂, c) C₂H₂, d) C₃H₃, e) C₄H₄, f) C₅H₅ with HAB.

Figure 10 (a) shows the relationship between mole fraction of OH (with 0%, 20% and 40% CO additive) and HAB. Figure 10 (a) showed that as the CO additive accelerates the forward reaction with OH and decreased the mole fraction of OH. So, in result the mole fraction of OH becomes lower with CO addition. The following reactions take place:

$$CO + OH \rightarrow CO_2 + H$$
 (15)

Figure 10 (b) shows the relationship between mole fraction of H₂ (with 0%, 20% and 40% CO additive) and HAB. It shows that the concentration of H₂ gradually increases with HAB. As the CO additive accelerates the forward reaction with H₂. So, in result the mole fraction of H₂ becomes lower with CO addition. In Figure 10 (c) the relationship between mole fraction of C₂H₂ (with 0%, 20% and 40% CO additive) and HAB is shown. CO doesn't react with C₂H₂ but it will react with other species and affect the result. Hence, the dilution effect is observed upon adding CO to hydrocarbon fuel flame. So when 20% to 40% CO was added to C₂H₂/air flame, the mole fraction of C₂H₂ decreased. Figure 10 (d) depicts the relationship between mole fraction of C₃H₃ (with 0%, 20% and 40% CO additive) and HAB. Carbon monoxide caused dilution effect on hydrocarbon fuel flame. So when 20% to 40% CO was added to C₂H₂/air flame, the mole fraction of C₄H₄ (with 0%, 20% and 40% CO additive) and HAB. The addition of CO to hydrocarbon fuel flame yields several effects, including dilution, thermal, chemical effects, etc. So when 20% to 40% CO was added to C₂H₂/air flame, the mole fraction of C₄H₄ decreased. On the whole, the concentration of C₄H₄ first increased sharply and then decreased to a flat state with HAB. Figure 10 (4) illustrates the relationship between mole fraction of C₅H₅ (with 0%, 20% and 40% CO additive) and HAB. The dilution effect is because of the addition of CO to hydrocarbon fuel flame. So when 20% to 40% CO was added to C₂H₂/air flame, the dilution effect is because of the addition of CO to hydrocarbon fuel flame. So when 20% to 40% CO additive) and HAB. The dilution effect is because of the addition of CO to hydrocarbon fuel flame decreased to a flat state with HAB. Figure 10 (4) illustrates the relationship between mole fraction of C₅H₅ (with 0%, 20% and 40% CO additive) and HAB. The dilution effect is because of the addition of CO to hydrocarbon fuel flame. So wh



Fig. 10: Mole Fractions of a) OH, b) H₂, c) C₂H₂, d) C₃H₃, e) C₄H₄, f) C₅H₅ with HAB.

Figure 11 (a) illustrates the relationship between mole fraction of OH (with 0%, 20% and 40% N₂ additive) and HAB. This is a forward reaction which consumes OH radical and due to which the mole fraction of OH started to decrease. Therefore, first the mole fraction of OH started to increase and after getting the maximum peak, the mole fraction of OH was started to decrease. It can clearly be seen that the results are very close to each other with two fluctuations (one is when reaction started and the other is after moving from maximum values). In other words, it is showing same trend with 0%, 20% and 40% N₂ addition. Figure 11 (b) elucidates the relationship between mole fraction of H₂ (with 0%, 20% and 40% N₂ additive) and HAB. When N_2 is added in C_2H_2/air flame, then it can be understanding that, mole fraction of H_2 was maximum with 0% N₂ and it was minimum with 40% N₂. Furthermore, it was in between the minimum and maximum value, when N₂ was 20%. In other words, it is showing the decreasing trend with 0%, 20% and 40% N_2 addition, because nitrogen is an inert gas but it effects the results due to dilution effect. Figure 11 (c) illustrates the relationship between mole fraction of C_2H_2 (with 0%, 20% and 40% N_2 additive) and HAB. It can clearly be seen that the results are very close to each other. In other words, it is showing same trend with 0%, 20% and 40% N₂ addition and lowering the mole fraction of C₂H₂, and for all percentages addition of N_2 decreased the mole fraction of C_2H_2 because nitrogen is an inert gas but it effects the results due to diffusion effect. Figure 11 (d) illustrates the relationship between mole fraction of C_3H_3 (with 0%, 20% and 40% N_2 additive) and HAB. It can clearly be seen that the end results are very close to each other. In other words, it is showing same trend with 0% and 20% N_2 but for 40% N_2 addition it showed a fluctuation and lowering the mole fraction of C_3H_3 . Figure 11 (e) illustrates the relationship between mole fraction of C_4H_4 (with 0%, 20% and 40% N_2 additive) and HAB. It can clearly be seen that the end results are close to each other for 0% and 20% of N_2 addition as compared to 40% N_2 addition. In other words, it is showing same trend with 0% and 20% N_2 , but for 40% N_2 addition it showed different and increased the mole fraction of C_4H_4 at high flame height. Figure 11 (f) is showing the relationship between mole fraction of C_5H_5 (with 0%, 20% and 40% N_2 additive) and HAB. It is clearly mentioned that the mole fraction of C_5H_5 started to increase from 0.2cm, when the percentage of N_2 was 0% and 20% it increased with same trend as seen in the figure. But for 40% addition of N_2 case, it shows a bit different pathway. Before HAB= 1.5cm, the concentration of C_5H_5 under 40% N_2 addition was much lower than that under other conditions, but higher after that.



Fig. 11: Mole Fractions of a) OH, b) H₂, c) C₂H₂, d) C₃H₃, e) C₄H₄, f) C₅H₅ with HAB.

Soot Volume Fraction:

To study the effects of H_2 , CO and N_2 on formation of soot, 0% to 40% H_2 , CO, N_2 were added in acetylene flame. In Figure 12 (a), (b), (c) showed that the soot formation reduced by the addition of H_2 , CO, N_2 .



Fig. 12: Soot Volume Fraction with HAB.

4. Conclusion

For the study of PAHs and soot volume fraction, CHEMKIN software was used to analyse the behaviour of H_2 , CO and N_2 , addition on the PAHs and soot production in a premixed laminar C_2H_2 flame numerically. For the detail clarification of impact of additives on PAH formation and intermediate species like OH, H_2 and C_2H_2 , C_3H_3 , C_4H_4 , C_5H_5 and soot volume fraction, some simulations were performed under different addition ratios (0%, 20% and 40%) of H_2 , CO and N_2 . The ABF mechanism which includes C_1 and C_2 chemistry, benzene, PAH growth was used in the simulation to understand the particle inception and mole fractions of intermediate species. The main concluding contents are:

1.Carbon monoxide and Nitrogen showed diluents effects the PAH and reduced the PAH due to dilution. Hydrogen addition showed the chemical effect when added to fuel side and PAH were inhibited significantly as compared to carbon monoxide and nitrogen. By the addition of H_2 a strong chemical effect on formation of A4 was observed and low mole fraction of A4 can be observed in flame of $C_2H_2/H_2/air$. Meanwhile, due to the abundance of H_2 the aromatic radicals are restricted thus resulting in low production rate of larger PAHs. Hence among all these additives, to reduce PAH formation H_2 can be a good additive.

2.At 0% addition of H_2 , CO and N_2 in C_2H_2 , the maximum temperature was 1742 K. By increasing the concentration of H_2 , CO and N_2 in C_2H_2 the temperature decreases and for 20% concentration of H_2 , CO and N_2 it reduced to 1710 K, 1719 K and 1725 K respectively. Similarly, for 40% concentration of H_2 , CO and N_2 , the temperature reduced to 1682 K, 1691 K and 1710 K respectively. This showed that these all additives have thermal effect. Hydrogen had a significant effect due to its chemical effect. CO is also having thermal effect but N_2 showed fewer change in temperature due to its inert nature.

3.Carbon monoxide and Nitrogen showed diluents effects when added to fuel side and the mole concentrations of soot predecessor species for example C_2H_2 reduced due to dilution. The addition of CO reduces the concentration of C_2H_2 . Hydrogen addition showed the chemical effect when added to fuel side and the mole concentrations of soot ancestor species like C_2H_2 were inhibited remarkably when compared to carbon monoxide and nitrogen. A strong chemical effect is observed in lowering the concentration of C_2H_2 in the $C_2H_2/H_2/air$ flame by adding H_2 .

4.Carbon monoxide and Nitrogen showed diluents effects and soot volume fraction reduced due to dilution. Hydrogen addition showed the chemical effect when added to fuel side and the soot volume fraction were decreased significantly as compared to carbon monoxide and nitrogen. Hence among all these additives, H_2 is an effective additive in lowering the formation of soot.

References

- [1] G. D. J. Guerrero Peña, Y. A. Hammid, and A. Raj, "On the characteristics and reactivity of soot particles from ethanolgasoline and 2, 5-dimethylfuran-gasoline blends," *Fuel*, vol. 222, pp. 42–55, 2018.
- [2] Y. Liu, Y. Gao, and N. Yu, "Particulate matter, gaseous and particulate polycyclic aromatic hydrocarbons (PAHs) in an urban traffic tunnel of China: Emission from on-road vehicles and gas-particle partitioning," *Chemosphere*, vol. 134(5), pp. 52–59, 2015.
- [3] H. Guo, K. A. Thomson, and G. J. Smallwood, "On the effect of carbon monoxide addition on soot formation in a laminar ethylene/air co-flow diffusion flame," *Combustion and Flame*, vol. 156(6), pp. 1135–1142, 2009.
- [4] Ö. L. Gülder, "Influence of hydrogen addition to fuel on temperature field and soot formation in diffusion flames," *Symposium on Combustion*, 1996.
- [5] A. Choudhary and S. Gollahalli, "Combustion characteristics of hydrogen-hydrocarbon hybrid fuels," *Hydrogen Energy*, vol. 25, pp. 451–462, 2000.
- [6] R. Henríquez, R. Demarco, J. L. Consalvi, F. Liu, and A. Fuentes, "The oxygen index on soot production in propane diffusion flames," *Combust. Sci. Technol*, vol. 186 (4–6), pp. 504–517, 2014.
- [7] A. D'Anna, "Detailed Kinetic Modeling of Particulate Formation in Rich Premixed Flames of Ethylene," *Energy & Fuels*, vol. 22, pp. 1610–1619, 2008.
- [8] M. Frenklach, "Method of moments with interpolative closure," Chem Eng Sci, vol. 57, pp. 2229–2239, 2002.
- [9] J. Appel, H. Bockhorn, and M. Frenklach, "Kinetic modeling of soot formation with detailed chemistry and physics: laminar premixed flames of C2 hydrocarbons," *Combust Flame*, vol. 121, pp. 122–136, 2000.
- [10] M. Frenklach, H. Wang, and H. Bockhorn, "Soot formation in combustion: mechanisms and models," *Springer-Verlag, Heidelberg*, pp. 165–192.
- [11] R. J. Kee, F. M. Rupley, and J. A. Miller, "Chemkin-II: A fortran chemical kinetics package for the analysis of gasphase chemical kinetics," *Sandia Rep*, pp. SAND89-8009B, 1989.
- [12] A. J, H. Bockhorn, and M. Wulkow, "A detailed numerical study of the variation of soot particle size distributions in laminar premixed flames," *Chemosphere*, vol. 42, pp. 635–645, 2001.