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Simulation Analysis on the Identification of Chemical Effects by the Addition of Diatomic Gases in Acetylene Flame

Hassan Osaf Ali[1], Daisuke Shimokuri[2], Muhammad Hassaan Athar[3], Faheem-ul-Hasnain[4], Talha Nadeem Hassan[5], Muhammad Azeem Ghouri[6]
[1]Hiroshima University
Hiroshima, Japan
d213219@hiroshima-u.ac.jp; cri@hiroshima-u.ac.jp
[1]Hiroshima University
Hiroshima, Japan

Abstract **-** In order to study the chemical effects by the addition of diatomic gases on PAHs, CHEMKIN software was used for the analysis of H_2, CO and N_2 effects on the PAHs in a premixed laminar C_2H_2 flame numerically. 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. To investigate the chemical effect, some simulations were done with new species which have same thermal and transport properties like H_2, CO, N_2 but the new species can't not participate in the chemical reactions. The results showed a significant difference on the mole fractions of aromatic species when the new added species compared with additives due to chemistry and the results showed that N_2/CO/H_2 restrict the PAH formation while new species (H_2*, CO*, N_2*) increased the PAH formation due to lack of chemical reactions. However, hydrogen showed strong chemical effect when it is added into the unburned mixture.
Keywords**:** H_2/CO/N_2 addition; Polycyclic Aromatic Hydrocarbon; Premixed Flame;

1. Introduction

Ongoing advancement in fuel improvement ignition and application of syngas animates our advantage in the impact of carbon monoxide (CO) addition on different flame properties, since CO is an essential part of a reformate gas or a syngas which is a compelling and useful advancement addictive substance [1]. Soot and other various contaminated emissions discharges which result from hydrocarbon have been difficult for quite a while. Numerous analysts have been researching the soot development phase of some fuels in the beyond quite a while, such as petroleum gas, fuel, lamp oil and diesel [2-6]. In any case, CO takes an interest in synthetic responses that might impact soot production. Thusly, the expansion of CO might have complex impact on particulate matters. Arthur and Napier [7] noticed that the expansion of CO had a weakly suppressive impact on soot in methane flame, however didn't propose any clarification for the conduct. Zhao H [8] observed that fuel mixed with hydrogen can successfully diminish the soot emission in an immediate injection spark engine. It uncovered that addtion of hydrogen brings about a critical change in the compressibility of the fuel blend and could adjust the chemical species concentration during the ignition.

To disengage the synthetic impact from others, the paper additionally examines the alternative of nitrogen (N_2), which has comparable thermal and weakening impacts as CO since they have comparative thermal and transport properties. Nitrogen is inert for soot development and doesn't chemically effect.

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 compare them with new additives (named H_2*, CO*, N_2*) which have same thermal and transport properties. The last but not least objective was to use the model to numerically evaluate the formation of PAH in Laminar Premixed Burner Flame by using CHEMKIN software to advance the understanding of PAH formation mechanism.

2. 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 [10] and Figure 4 [10]. 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.

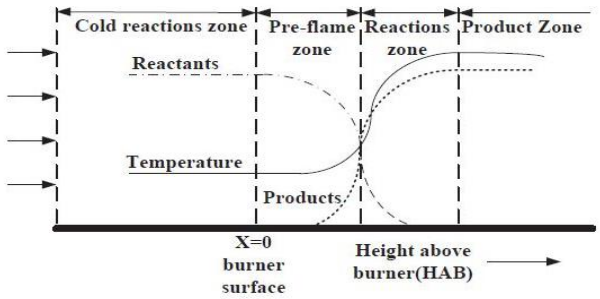


Fig. 1: Schematic of one-dimensional premixed flame configuration.

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.

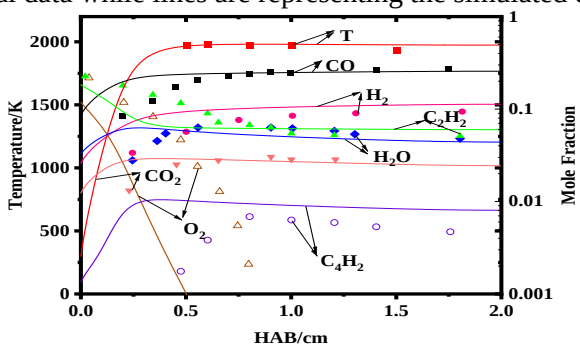


Fig. 2: Comparison of calculated and experimental data of mole fractions profiles for major products in pure C2H2/air flames [9] by ABF mechanism.

Figure 3 demonstrates the simulated mole fraction of benzene and naphthalene with the experimental data of previous studies [10]. It is clearly seen that the calculated date agreed well with experimental data of mole fractions of benzene and naphthalene with respect to HAB by using ABF mechanism.

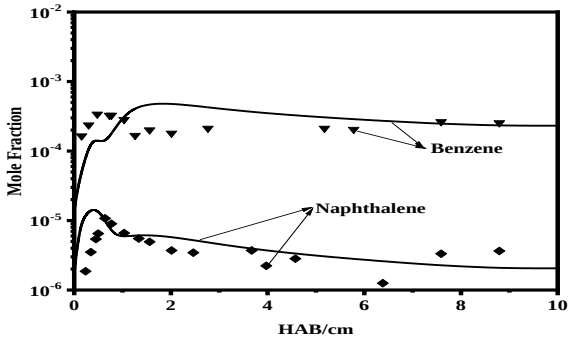


Fig. 3: Comparison of calculated and experimental data [12] of PAH in pure C_2H_2/air flames by ABF mechanism.

2.1. Boundary Conditions

The following tables 1 and 2 represent the calculation conditions for the simulation of C_2H_2/air Flame.

Table 1: Calculation conditions for C2H2/air Flame.

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

Table 2: Calculation conditions for C2H2/air Flame.

H_2, CO, N_2 (Volume)	0%	20%	30%
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

3. Results and Discussion

Identification of Chemical Effect:

To investigate the chemical effect, some new species (named H_2*, CO*, N_2*) were added into the mechanism. These species have the same thermal and transport properties as the normal gases (H_2, CO, N_2), but they don't participate in the chemical reactions. The new species were adopted to simulate the flames and the results were compared with those for normal cases.

Figure 4 is depicting the mole fraction of A1 with respect to HAB. It is clearly seen at 0% condition, the mole fraction of A1 is minimum at the higher flame height. When we added 20% H_2, the mole fraction increases and the concentration is even higher than that at 20% H_2* addition condition. Therefore, it is concluded that the addition of H_2 has significant chemical effect in increasing the mole fraction of A1. Figure 4 is demonstrating the mole fraction of A2 with respect to HAB. It is clearly seen at 0% condition, the mole fraction of A2 is minimum at the high flame height. When we added 20% H_2, the mole fraction of A2 increases. However, adding 20% H_2* into the flame obviously increases the concentration A2 more significantly. Then it is concluded that the addition of H_2 chemically promotes the generation of A1, however inhibits the production of A2. Figure 4 is demonstrating the mole fraction of A3 with respect to HAB. It is clearly seen at 0% condition, the mole fraction of A3 is minimum at the high flame height. When we added 20% H_2, the mole fraction of A3 increases. Similarly, with the variation of A2, the addition of H_2* can promote the generation of A3 more significantly. Then it is concluded that the addition of H_2 can chemically promote the generation of A3. Figure 4 is demonstrating the mole fraction of A4 with respect to HAB. It is clearly seen at 0% condition, the mole fraction of A4 keep increasing. When we added 20% of H_2 the mole fraction of A4 decreases and by comparing it with new added specie which H_2*, then it is concluded that the addition of H_2 significantly reduces the mole of fraction of A4 due to its chemical effect.

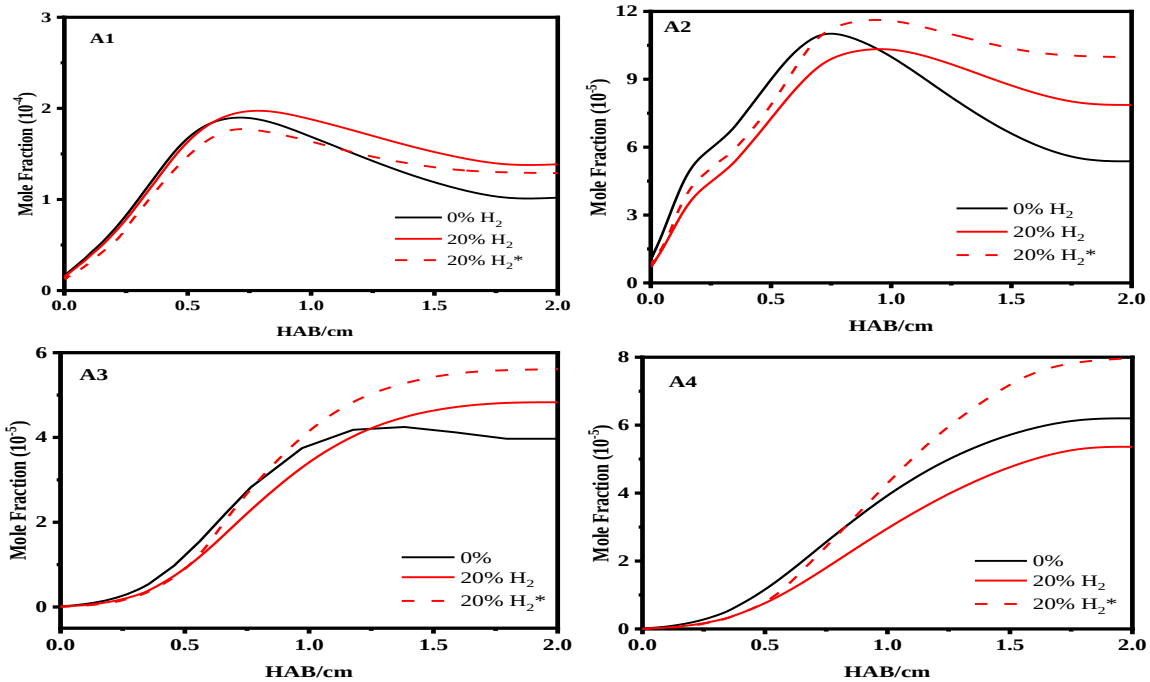
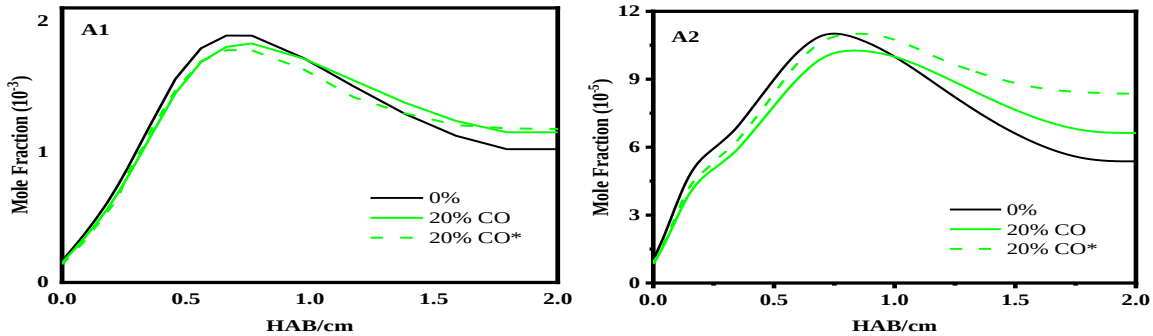


Fig. 4: Mole Fraction (a)A1, (b)A2, (c)A3, (d)A4 with HAB.

Figure 5 is depicting the mole fraction of A1 with respect to HAB. It is seen the mole fraction of A1 is the increased when added 20% CO into ethylene flame at high flame height. By comparing it with new added specie condition, it is concluded that the addition of CO has slight effect in decreasing the mole fraction of A1. Figure 5 is demonstrating the mole fraction of A2 with respect to HAB. It is clearly seen the mole fraction of A2 is minimum at 0% CO condition. When 20% CO is added into the flame, the mole fraction of A2 increases. When 20% CO* is added into the flame, the mole fraction of A2 further increases. Through the comparison, it is concluded that the addition of CO can chemically decrease the production of A2. Figure 5 is demonstrating the mole fraction of A3 with respect to HAB. It is clearly seen the mole fraction of A3 is increasing at 20% addition of CO. When added 20% CO* into the flame, the mole fraction increases more than CO addition case. Through the comparison, it is concluded that the addition of CO can chemically inhibit the production of A3. Figure 5 is showing the mole fraction of A4 with respect to HAB. It is clearly seen the mole fraction of A4 is increasing at 20% addition of CO* condition. When added 20% CO the mole fraction decreases significantly. Thus the addition of CO has significant effect in decreasing the mole fraction of A4.



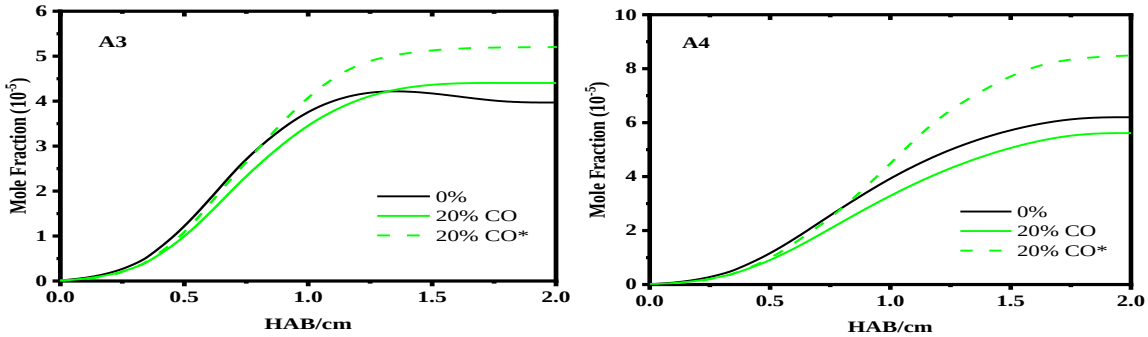


Fig. 5: Mole Fraction (a)A1, (b)A2, (c)A3, (d)A4 with HAB.

Figure 6 displays the mole fraction of A1 with respect to HAB. It is clearly seen the mole fraction of A1 is increasing at 20% addition of N_2*. When added 20% N_2, the mole fraction increased but less than N_2*. Thus the addition of N_2 has chemical effect on decreasing A1. Figure 4-24 is representing the mole fraction of A2 with respect to HAB. It is clearly seen the mole fraction of A2 is increasing at 20% addition of N_2*. When added 20% N_2, the mole fraction increased but less than N_2*. Thus the addition of N_2 has effect in decreasing the mole fraction of A2. Figure 6 is representing the mole fraction of A3 with respect to HAB. It is clearly seen the mole fraction of A3 is increasing at 20% addition of N_2*. When added 20% N_2, the mole fraction increased but less than N_2*. Thus the addition of N_2 has effect in decreasing the mole fraction of A3. Figure 6 is representing the mole fraction of A4 with respect to HAB. It is clearly seen the mole fraction of A4 is decreased for 20% addition of N_2. When added 20% N_2*, the mole fraction increased. By comparing the effect of new specie with N2, it is concluded that the addition of N_2 has effect in decreasing the mole fraction of A4.

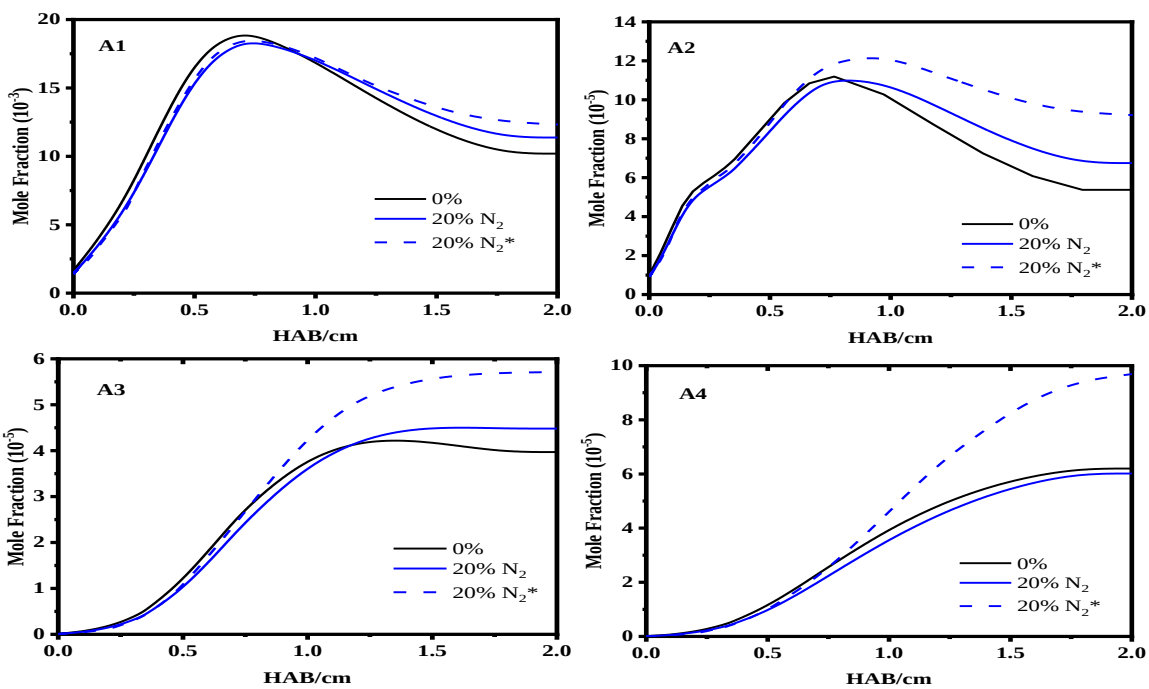


Fig. 6: Mole Fraction (a)A1, (b)A2, (c)A3, (d)A4 with HAB.

4. Conclusion

For the study of PAHs, CHEMKIN software was used to analyse the behaviour of H_2, CO and N_2, addition on the PAHs in a premixed laminar C_2H_2 flame numerically. The main concluding contents are:

To investigate the chemical effect, some simulations were done with new species which have same thermal and transport properties like H_2, CO, N_2 but the new species can't not participate in the chemical reactions. The results showed a significant difference on the mole fractions of aromatic species when the new added species compared with additives due to chemistry and the results showed that N_2/CO/H_2 restrict the PAH formation while new species (H_2*, CO*, N_2*) increased the PAH formation due to lack of chemical reactions. However, hydrogen showed strong chemical effect when it is added into the unburned mixture.

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