Chemical Effects of CO₂ Concentration on Flame Structure and Soot Precursors in Rich Ethylene Oxidation

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Flame structure and soot precursors were investigated numerically with CO₂ addition in fuel enrichment laminar premixed C₂H₄/O₂/Ar flames (C/O ratio of $\Phi = 2.5$) at low pressure (0.05 atm). An updated mechanism emphasizes the effect of presence of an O₂/CO₂ atmosphere instead of an O₂/Ar one in premixed flame. The addition of CO₂ in the fresh gas inlet causes a shift downstream of the flame front and thus flame inhibition. The partial replacement of Ar by CO₂ leads to an increase of burnt gas quantities of H₂O, CO and CO₂ and leads to a decrease of the maximum mole fractions of some C₂ to C₁₀ hydrocarbon intermediates (C₂H₂, C₃H₃, C₆H₆, C₆H₆O, C₈H₈ and C₁₀H₈). The sensitivity analysis and reaction-path analysis show that C₂H₄ reaction path and products are altered due to the CO₂ addition.

Key Words: Fuel enrichment, Carbon dioxide, Kinetics modeling, Flame structure, Soot precursors.

INTRODUCTION

Exhaust gas recirculation systems and oxy-fuel burners with CO₂ recycling have been used successfully in a number of industrial processes and shown to improve combustion efficiency and reduce pollutant emissions. However, these industrial processes are mostly accompanied by NO_x and soot particles emission which have a detrimental effect on human health and contribute significantly to global warming¹⁻³. So, the radiative properties of oxy-fuel flames and the role of soot is a persistent problem in many processes that involve fuel-rich combustion of hydrocarbon fuels⁴.

A number of investigations have been focused on reducing soot emission by introducing several techniques, including the use of different fuels and addition of diluents on the oxidizer or fuel side in diffusion flames. Especially, study of the effect of CO₂ additives on soot emission has been a special interest for suppressing soot production tendency, such as those by Ni and co-workers⁵ and Liu and co-workers⁶. These investigations found that the addition of CO₂ on either fuel side or oxidizer has chemical effects on soot formation reduction, which might be to promote the concentrations of oxygen atom and hydroxyl that in return increase the oxidation of soot precursors in soot formation regions, in addition to dilution and thermal effects.

Recently two experimental investigations have been conducted by Renard *et al.*⁷ and Vandooren *et al.*⁸ on CO₂ addition to rich C₂H₄/O₂/Ar and CH₄/O₂/Ar premixed flames. The

results showed that CO₂ and H₂O addition are responsible for reduction of hydrocarbon intermediates in flames. It has been established experimentally that addition of CO₂ suppresses soot emission chemically in both diffusion and premixed flames. However, the chemical effects of CO₂ addition on flame structure in premixed flames remains unclear, especially for computation investigation.

The main objective of this study is to numerically investigate the mechanism of the chemical effect of CO₂ addition on the structure of premixed rich C₂H₄/O₂/Ar(N₂) flames at low pressure and atmospheric pressure. An updated mechanism of C₂H₄/air combustion based on Kazakov *et al.*³ with emphasis on CO₂ addition was modified from previous studies in the literature. The main combustion concentration profiles have been predicted using the updated mechanism and verified against the experimental data. The test conditions were limited to fuel-rich laminar premixed ethylene/air flames at low pressure and different C/O ratios, similar to the flames studied by Renard⁷ and Vandoorens⁸. To further understand the effect of CO₂ addition on soot formation at atmospheric pressure. The kinetic models were scrutinized with sensitivity, rate of production analysis and path of reaction analysis.

Combustion mechanisms and simulation

Reaction mechanism without CO₂ additive: In this article, the gas-phase original comprehensive reaction mechanism was developed by Kazakov and co-workers³ for

the oxidation of C₂H₄ in air combustion. The detailed chemical kinetic model consisted of 680 reactions and 156 species. Calculation was performed using the Premixed Laminar Model of the CHEMKIN-PRO package. Thermodynamic properties were obtained from CHEMKIN database. Transport properties were obtained from the Sandia CHEMKIN transport data base⁹. Some species were predicted and verified against the experimental data in premixed C₂H₄/O₂/Ar without CO₂ addition at low pressure.

The main species involving soot precursors are discussed in detail, such as reactants, products, acetylene, benzene, pyrene and so on. The role of resonantly stabilized radicals were investigated in aromatic, branched aromatic and polycyclic aromatic hydrocarbon formation in a premixed, rich, laminar, C₂H₄/O₂/Ar flame.

Reaction mechanism with CO₂ additive: The computed results on polycyclic aromatic hydrocarbon formation for C₂H₄ oxidation in different O₂/CO₂ atmospheres are analyzed in terms of a gas-phase chemical kinetic model, which was updated from the mechanism of Kazakov and co-workers³. This mechanism provides in general reasonably good agreement between modeling and experimental results, even though some modifications are needed to take into account the effect of the presence of high CO₂ concentration levels. An updated mechanism was developed to identify the chemical effects of an additive (CO₂) introduced to the fuel mixture. Therefore, in the present work, the mechanism has been updated, with particular emphasis on the effect of the presence of an O₂/CO₂ atmosphere instead of air or O₂/Ar. A number of reactions involving CO₂ species which do not appear in the initial model but may be important during the C₂H₄ oxidation process under oxy-fuel conditions have been included. Moreover, revisions of rate constants of the most sensitive reactions in the mechanism under the specific conditions studied were modified based on previous studies in the literature. These modifications and the main reactions of interest are performed as an attempt to attain a better prediction of the experimental data. The modifications are listed in Table-1. These modifications

and the main reactions of interest are described below. Calculations are performed using the PREMIX model. The reverse rate constants were taken from the same source as the mechanism.

In order to establish the reaction mechanism, the conversion of CO₂ to CO (Table-1) needs to be emphasized for activating chemically the comparatively inert CO₂ molecule. The strong carbon-oxygen double bonds in CO₂ need to spend high temperature or very reactive free radical breaking it.

The reaction of thermal dissociation for CO₂

which occurs only at high temperatures with strongly endothermic. The most important reaction with atomic hydrogen

is comparatively fast even at medium temperatures. This reaction would be the dominating reaction under combustion conditions for CO/CO₂ partial equilibrium. The rate constant for the reaction can be seen in¹⁰⁻¹⁹.

Reactions of other species with CO₂ from the O/H radical pool, *i.e.*:

are important because of slow.

The most abundant intermediate radical species is CH₃ for C₂H₄ combustion. The CH₃ may react with CO₂ to form CH₃O and CO

which reaction for the reverse direction, CH₃O + CO $\rightleftharpoons$ CH₃ + CO₂ (R11), shows little consistency²⁰ with available results. Wang *et al.*²¹ study results show that addition/elimination to CH₃ + CO₂ and direct H atom abstraction to CH₂O + HCO is important at higher temperatures. The overall rate constant which was calculated by Wang *et al.*²¹ indicates that lies above the low-temperature results of Koch *et al.*²² and below those of Wantuck *et al.*²³ at high temperatures. According to Rasmussen and Glarborg¹⁴, CH₃ + CO₂ is the sole product channel from CH₃O + CO and the result was adopted²⁴.

TABLE-1
REACTIONS SUBSET FOR CO₂

	Reactions	A [cm, mol, s]	β	E _a [cal/mol]	Ref.
1	CO+O(+M) $\rightleftharpoons$ CO ₂ (+M ^a)	1.8 × 10 ¹⁰	0	2384	10,11
	Low-pressure limit:	1.4 × 10 ²⁴	-2.79	4191	11,12
2 ^b	CO+OH $\rightleftharpoons$ CO ₂ +H	8.0 × 10 ¹⁰	0	0	13
		8.8 × 10 ⁵	1.77	954	
3	CO+OH $\rightleftharpoons$ HOCO	2.0 × 10 ¹⁶	-5.6	2881	13
4	CO+HO ₂ $\rightleftharpoons$ CO ₂ +OH	1.0 × 10 ⁵	2.18	179400	14
5	CO+O ₂ $\rightleftharpoons$ CO ₂ +O	4.7 × 10 ¹²	0	60500	15
6	HOCO $\rightleftharpoons$ CO ₃ +H	3.5 × 10 ³⁶	-15	46500	13
		2.5 × 10 ⁶⁹	-18	60000	
7 ^b	HOCO+OH $\rightleftharpoons$ CO ₂ +H ₂ O	4.6 × 10 ¹²	0	-89	16
		9.5 × 10 ⁶	2	-89	
8	HOCO+OH $\rightleftharpoons$ CO ₂ +HO ₂	9.9 × 10 ¹¹	0	0	17
9	HCO+O $\rightleftharpoons$ CO ₂ +H	3.0 × 10 ¹³	0	0	18
10	HCO+HO ₂ $\rightleftharpoons$ CO ₂ +OH+H	3.0 × 10 ¹³	0	0	19
11	CH ₃ O+CO $\rightleftharpoons$ CH ₃ +CO ₂	9.5 × 10 ²⁵	-4.93	9080	20
12	³ CH ₂ +CO ₂ $\rightleftharpoons$ CH ₂ O+CO	1.0 × 10 ¹¹	0	1000	21
13	¹ CH ₂ +CO ₂ $\rightleftharpoons$ CH ₂ O+CO	1.1 × 10 ¹³	0	0	22
14	CH+CO ₂ $\rightleftharpoons$ HCO+CO	8.8 × 10 ⁶	1.75	-1040	28

^aEnhanced third-body efficiencies: H₂ = 2.5, H₂O = 12, CO = 1.9, CO₂ = 3.8. ^bExpressed as the sum of the constants.

Reactions of CO₂ with small hydrocarbon fragments include

The CH₂ radical has two existing states in combustion processes. Singlet methylene (³CH₂) is more reactive toward radicals than the triplet state (¹CH₂), but it reacts slower with stable molecules.

The measurement results show that reaction R12 is less than an order of magnitude slower reaction R13 (Table-1), but they are uncertain for the rate constants of these reactions.

The rate constant used for ³CH₂ + CO₂ relies on the room temperature measurement by Laufer and Bass²⁴ and the activation energy was assessed in the present work. Nevertheless, the most research results indicate that the reaction may be even slower in room temperature. For ¹CH₂ + CO₂ (R13), the early estimate by Tsang and Hampson¹⁹ under the room temperature shows a somewhat slower rate constant than the only experimental value by Koch *et al.*²².

In this paper, the data obtained from those research data and reasonable estimates for Arrhenius expression shown in Table-1.

The model assumes that nucleation of soot particles is due to the coalescence of two large size polycyclic aromatic hydrocarbon, pyrene (A4), into a dimer. Then the particle size increases or decreases due to the particle coagulation, surface growth and oxidation.

EXPERIMENTAL

First of all, the experimental data for three premixed flames at equivalence ratios in the range of 1.00-2.00 (1.00, 1.50 and 2.00) are obtained from Renard *et al.*²⁵ to validate the original model on a flame burner 8 cm in diameter at pressures varying from 0.03 to 0.05 atm. In addition, the experimental data of rich premixed C₂H₄/O₂/Ar flames for one without any additive (F2.50) and one with 15 % of CO₂ replacing the same quantity of argon (F2.50C) were obtained (Renard *et al.*⁷ and Ho and Chou²⁶ to investigate the effect of CO₂ on the premixed flame of C₂H₄). The mole detail about experimental data can be seen in Table-2.

RESULTS AND DISCUSSION

Without CO₂ addition in premixed C₂H₄/O₂/Ar flames:

The simulations were performed for three premixed flames at equivalence ratios in the range of 1.0-2.0 (1.0, 1.5 and 2.0) to test the original model on a flame burner 8 cm in diameter at pressures varying from 0.03-0.05 atm (Table-2). The simula-

tions of experimental data from Renard *et al.*²⁵, the molecular beam mass spectrometry (MBMS) measurements of species in a fuel-rich C₂H₄/O₂/Ar flame, are presented in Fig. 1. The predicted and experimental mole fraction of C₂H₄ and H₂ concentrations are shown in Fig. 1(a-b). The simulated concentrations of small molecules and radicals H₂ and C₂H₄ are in good agreement with the experimental data. In general, the maximum error of C₂H₄ and H₂ concentrations for three equivalence ratios are under-predicted by 13.3 %. In view of systematic errors in the measurement, this under-prediction can be accepted.

Fig. 1. Comparison of model predictions with experimental concentration profiles in the C₂H₄/O₂/Ar flame for various several equivalence ratio (Φ). (a) Comparison for C₂H₄. (b) Comparison for H₂.

Effect of CO₂ addition in premixed C₂H₄/O₂/CO₂/Ar flames: The computed results on polycyclic aromatic hydrocarbon formation for C₂H₄ oxidation in various O₂/CO₂/Ar atmospheres are analyzed in terms of a detailed gas-phase

TABLE-2
FLAME COMPOSITION AND COMPUTED CONDITIONS

Model	Flames	Φ	X(C ₂ H ₄)	X(O ₂)	X(Ar)	X(CO ₂)	P (atm)	v ₀ (cm/s)
Premix model	F1.0	1.0	0.0675	0.2025	0.7300	0	0.03	78.36
	F1.5	1.5	0.1012	0.2025	0.6963	0	0.04	58.79
	F2.0	2.0	0.1350	0.2025	0.6625	0	0.05	47.03
	F2.5	2.5	0.3300	0.4000	0.2700	0	0.05	40.3
	F2.5C	2.5	0.3300	0.4000	0.1200	0.1500	0.05	40.3

chemical kinetic model. The comprehensive reaction mechanism used as the starting mechanism for the modeling study was developed by Kazakov and co-workers³ for the oxidation of C₂H₄ in air combustion. An updated mechanism was developed to identify the chemical effects of an additive (CO₂) introduced to the fuel mixture. Therefore, the updated mechanism emphasizes the effect of the presence of an O₂/CO₂ atmosphere instead of air or O₂/Ar. The modifications are listed in Table-1. Calculations were performed using the PREMIX model. The reverse rate constants were taken from the same source as the mechanism. In this section, only temperature and mole fraction profiles of important species involving soot formation are discussed in detail.

The addition of CO₂ replacing an equivalent amount of argon (Table-2) to the rich ethylene flame F2.5 has led to several effects which are described below. The simulated and experimental temperature and mole fraction profiles of H₂O in F2.5 and F2.5C flames are shown in Fig. 2. The simulated results agree well with the experimental data, even if the predictions of temperature and H₂O mole fraction are a little higher than the experimental results for both F2.5 and F2.5C. According to Renard and co-workers²⁵, the difference is due to experimental uncertainties. Indeed, the replacement of some quantities of argon by equivalent amounts of CO₂ leads to a displacement of the flame front of 1-2 mm downwards and to an increase in the mean heat capacity. The partial replacement of Ar by CO₂ leads to an increase of burnt gases quantities of H₂O, CO and CO₂.

As it is illustrated in Figs. 2b and 3a, the presence of CO₂ in the fresh gases (F2.50C) induces larger yields of CO (17 %) and H₂O (25 %) through the overall reaction

For the doped flame (F2.50C), a decrease of the burning velocities was observed compared to the F2.50 flame, which consists of a shift of the flame front about 0.5-1.0 mm downstream from the burner surface as is easily observed through the mole fraction profiles of C₂H₄ (Fig. 3b). From Fig. 3b, the presence of CO₂ in the fresh gases (F2.50C) induces an increase of final quantities of CO₂ (37 %). Also, the simulated profiles of CO, CO₂, C₂H₂ and C₂H₄ agree well with the experimental ones (Fig. 3).

Fig. 4 shows the maximum mole fractions of some C₂ to C₁₀ species at equivalence ratio of 2.50. The simulated results agree well with the experimental data, even if the prediction of C₆H₆O is a little higher than the experimental result. CO₂ addition usually leads to a decrease by only about 5-20 % of

Fig. 2. Comparison of predicted profiles with the experimental profiles in the C₂H₄/O₂/Ar and C₂H₄/O₂/Ar/CO₂ flames at $\Phi = 2.5$. (a) Comparison for temperature. (b) Comparison for H₂O

the maximum mole fractions of some C₂ to C₁₀ hydrocarbon intermediates (C₂H₂, C₃H₃, C₆H₆, C₆H₆O, C₈H₈ and C₁₀H₈) (Figs. 3b and 4). The decrease of that of C₂H₂ is more marked in the flame F2.50C (30 %).

Sensitivity analysis and reaction path analysis: The C₂H₄/O₂/Ar(N₂) combustion mechanism of Kazakov and co-workers³ is used in the simulation. This reaction mechanism consists of 156 species and 680 reactions which include polycyclic aromatic hydrocarbon growth reactions up to pyrene, A4. The code names for some are shown in Table-3. According to Frenklach and co-workers¹⁰, soot particles are created by the dimerization of pyrene molecules.

TABLE-3
AROMATIC SPECIES

No.	Name	Structure	No.	Name	Structure
1	Phenyl, A1-	C ₆ H ₅	11	Naphthalene, A2	C ₁₀ H ₈
2	Benzene, A1	C ₆ H ₆	12	Biphenyl, P2	C ₁₂ H ₁₀
3	Toluene	C ₇ H ₈	13	Methylnaphthalene, A2CH ₃	C ₁₁ H ₁₀
4	Benzyl, C ₇ H ₇	C ₆ H ₅ CH ₂	14	Ethynylnaphthalene, A2C ₂ H	C ₁₂ H ₈
5	Phenyl acetylene, A1C ₂ H	C ₆ H ₅ C ₂ H	15	Acenaphthalene, A2R5	C ₁₂ H ₈
6	Ethynylphenyl radical, A1C ₂ H-	C ₆ H ₄ CCH	16	Phenanthrene, A3	C ₁₄ H ₁₀
7	Styrene, A1C ₂ H ₃	C ₆ H ₅ C ₂ H ₃	17	Methylphenanthrene	C ₁₄ H ₁₂
8	Phenylvinyl radical, A1C ₂ H ₃ *	C ₆ H ₄ CH=CH ₂	18	Phenanthrylacetylen, A3C ₂ H	C ₁₆ H ₁₀
9	<i>n</i> -Styryl, <i>n</i> -C ₈ H ₇	C ₆ H ₅ CH=CH	19	Pyrene, A4	C ₁₆ H ₁₀
10	Indene	C ₉ H ₈	20	Pyreneacetylene, A4C ₂ H	C ₁₈ H ₁₀

Fig. 3. Comparison of predicted mole profiles of main C_1 -, C_2 -species with the experimental profiles in the $\text{C}_2\text{H}_4/\text{O}_2/\text{Ar}$ and $\text{C}_2\text{H}_4/\text{O}_2/\text{Ar}/\text{CO}_2$ flames at $\Phi = 2.5$. (a) Comparison for CO_2 and CO . (b) Comparison for C_2H_4 and C_2H_2 .

Fig. 4. Comparison of maximum prediction of mole profiles of main C_3 - C_{10} species (C_3H_3 , C_6H_6 , $\text{C}_6\text{H}_6\text{O}$, C_8H_8 and C_{10}H_8) with the experimental profiles in the $\text{C}_2\text{H}_4/\text{O}_2/\text{Ar}$ and $\text{C}_2\text{H}_4/\text{O}_2/\text{Ar}/\text{CO}_2$ flames at $\Phi = 2.5$.

According to the mechanism (Fig. 5a), the most important consumption reaction of ethylene is $\text{C}_2\text{H}_4 + \text{H} = \text{C}_2\text{H}_3 + \text{H}_2$ which is the main route for the formation of vinyl radicals. This C_2H_3 radical leads to the formation of acetylene (C_2H_2) by decomposition. Acetylene is an important compound since

Fig. 5. Comparison of sensitivity analysis without and with CO_2 additive in the $\text{C}_2\text{H}_4/\text{O}_2/\text{N}_2$ flames at $\Phi = 2.2$.

it has been recognized as an important precursor for soot formation. Indeed, C_2H_2 allows the formation of C_3 and C_4 hydrocarbons. The main formation of propargyl radicals comes from the reaction of acetylene with singlet methylene radicals: $\text{C}_2\text{H}_2 + {}^1\text{CH}_2 = \text{C}_3\text{H}_3 + \text{H}$. Moreover, C_3H_3 can be produced from propyne and allene by hydrogen abstraction. The combination of resonantly stabilized free radicals such as propargyl, allyl, 1-methylallenyl and cyclopentadienyl were identified as an important aromatic and polycyclic aromatic hydrocarbon precursor species which eventually lead to benzene, toluene, xylene, naphthalene and phenanthrene formation in flames. These resonantly stabilized radicals play an important role in aromatic and polycyclic aromatic hydrocarbon formation as these species can build up in concentration within the flame since they are relatively resistant to oxidation by O_2 .

The important steps in soot formation from gas phase hydrocarbons are believed to be formation of the first ring, formation of polycyclic aromatic hydrocarbons (PAHs), soot inception and subsequently soot growth. It is now widely accepted that benzene and phenyl formation constitutes the first step in this growth process that lead to polycyclic aromatic hydrocarbon and ultimately soot particles. However, despite the extensive work on the elementary reactions leading to the

first aromatic ring, neither the dominant benzene (C₆H₆, A1) formation pathway nor the sensitivity of benzene (C₆H₆, A1) in C₂H₄/O₂/N₂ and C₂H₄/O₂/CO₂ atmosphere is yet well understood.

Fig. 5 shows the results of C₆H₆ (A1) normalized sensitivity coefficients of 17 reactions for C₂H₄/O₂/N₂ (Fig. 5a) and C₂H₄/O₂/CO₂ (Fig. 5b) flames at 1 atm and temperature 1630 K. There are three reactions (R234, R224 and R193) at 1630 K:

which have absolute values of sensitivity coefficients that are larger in both flames. However, there are some reactions that are different in the two flames; such as R451, R375, R239, R369, R152, R89, R69, R60 and R2. These nine reactions appear in Fig. 5a but are replaced by R257, R205, R85, R76, R75, R73, R31, R3 and R1 in Fig. 5b. So, the C₂H₄ oxidation is changed due to CO₂ addition. Some reactions that have higher sensitivity coefficients are not presented here.

Finally, the typical reaction-path diagrams in Fig. 6 represent the main reactions and species leading to benzene formation in C₂H₄/O₂/N₂ atmosphere (Fig. 6a) and C₂H₄/O₂/CO₂ atmosphere (Fig. 6b). Such diagrams, resulting from combining Fig. 5, are useful in identifying the difference in benzene formation in the different atmospheres. In Figs. 6a-b, the hydroxide radical (OH), oxygen radical (O) and other side species (H) are chosen as side species. Any reaction with the hydroxide radical is coloured purple, any reaction with the oxygen radical is coloured green and any reaction with H is coloured black. Each substantial reaction is represented by an arrow, the thickness of which is representative of the relative importance of that particular reaction of formation. The diagrams are not representative of all reactions in the mechanism but only concern the main pathways leading to benzene formation.

From Fig. 6, benzene formation is mainly achieved in two ways: C₂H₂ → C₃H₃ → A1(C₆H₆) and C₂H₂ → A1(C₆H₆) in both C₂H₄/O₂/N₂ and C₂H₄/O₂/CO₂ atmosphere. From Fig. 6a, besides conversion of small amounts to CO, most of the C₃H₃ converts to A1 in C₂H₄/O₂/N₂ atmosphere. However, besides most of the C₃H₃ converting to A1 and CO, a certain amount of C₃H₃ converts to HCO in Fig. 6b. So, this is a factor that the soot volume fraction decreases in the C₂H₄/O₂/CO₂ flame compared to the C₂H₄/O₂/N₂ flame. Comparing Figs. 6a-b, there are different main paths between the two. They are C₂H₄ → C₂H₂ → C₄H₂ → i-C₄H₂ → CH₂CO → CO₂, C₂H₄ → C₂H₂ → C₄H₂ → i-C₄H₂ → CH₂CO → CH₃ → CH₄ in the C₂H₄/O₂/N₂ flame (Fig. 6a) and C₂H₄ → C₂H₂ → C₄H₂ → H₂C₄O → CH₂CO → CH₃ CH₂O → HCO in the C₂H₄/O₂/N₂ flame (Fig. 6b). It can be concluded that CO₂ in the atmosphere changed the path of C₂H₄ oxidation.

Conclusion

A kinetic modeling study was carried out to investigate the mechanism of the chemical effects of CO₂ addition on the flame structure in a premixed flame under a pressure of 0.05 atm at equivalence ratios $\Phi = 2.5$. An updated mechanism, which was applied and shown to reproduce reasonably well the concentration profiles of major, intermediate and aromatic

Fig. 6. Comparison of reaction analysis without and with CO₂ additive in the C₂H₄/O₂/N₂ flames at $\Phi = 2.2$

species in ethylene flames, focused on the effect of the presence of an O₂/CO₂ atmosphere instead of air or O₂/Ar. Numerical results were verified against experimental data. Modeling predictions of reactants, stable intermediates and polycyclic aromatic hydrocarbon compounds generally showed good agreement with experimental data.

The addition of CO₂ in the fresh gas inlet causes a shift downstream of the flame front and thus flame inhibition, in the premixed C₂H₄/O₂/CO₂/Ar flame. The partial replacement of Ar by CO₂ leads to an increase in burnt gases quantities of H₂O, CO and CO₂ and leads to a decrease in the maximum mole fractions of some C₂ to C₁₀ hydrocarbon intermediates (C₂H₂, C₃H₃, C₆H₆, C₆H₆O, C₈H₈ and C₁₀H₈).

The sensitivity analysis and reaction-path analysis were conducted for C₂H₄/O₂/N₂ and C₂H₄/O₂/N₂/CO₂. The results show that C₂H₄ reaction path and products are altered due to the CO₂ addition.

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