



Effects of C_2H_2 and C_2H_4 radiation on soot formation in ethylene/air diffusion flames

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ABSTRACT

The involvement of hydrocarbons such as C_2H_4 and its combustion intermediate species C_2H_2 in thermal radiation has not been accounted in the numerical simulations of literature studies, which may in turn cause errors in estimating the soot formation processes. Numerical calculations were conducted using detailed gas-phase chemistry and thermal and transport properties in laminar coflow ethylene/air diffusion flames. The SNBCK model parameters for C_2H_2 and C_2H_4 were generated based on HITRAN database. The results show that the position of soot formation is affected by the radiation absorption of C_2H_4 at low temperatures and the radiation emission of C_2H_2 at high temperatures. The maximum C_2H_2/C_2H_4 radiation effect is 9.46% for air condition case and 9.87% for oxygen-enriched case. The height corresponding to the maximum soot volumetric fraction increases for the air condition while it decreases for the oxygen-enriched condition when the radiation effect is considered. The calculations reproduced well the experimental data of soot volumetric fraction in the literature and the numerical results were improved by 10.4% when considering the C_2H_2/C_2H_4 radiation. The results indicate that the radiation heat transfer of C_2H_2 and C_2H_4 needs to be taken into account in the numerical modeling of the ethylene/air diffusion flames.

1. Introduction

Gas thermal radiation plays an important role in the heat transfer and soot formation of combustion systems [1]. Due to the difficulty in solving the radiative transfer equation (RTE) in multidimensional geometry and the hyperspectral dependence of the absorption coefficient on the radiation gas [2–5], it is challenging to calculate the heat radiation transfer accurately and efficiently.

Ethylene laminar diffusion flame is a canonical problem in the study of radiation heat transfer in flames, because of its simple chemistry, moderate soot formation, and suitability for experiments under laboratory conditions [6,7]. Kaplan et al. [8] first considered radiation effects of soot, H_2O and CO_2 on the soot formation in ethylene diffusion flames. Liu et al. [9,10] studied the radiation heat transfer in counterflow and coflow ethylene laminar diffusion flames based on a detailed chemical reaction mechanism, a soot model and the statistical narrow-band correlated-k (SNBCK) model. They found the peak soot volumetric fraction increased by 8% when the gas radiation was ignored, and the radiation effect on soot nucleation and growth was larger than that on soot oxidation [10]. Subsequently, Guo and Smallwood [11,12] added

CO_2 and H_2 in ethylene/air laminar diffusion flames to study the chemical and radiation effect of CO_2 and H_2 on soot inception and surface growth rates. However, the role of ethylene (C_2H_4) and its combustion intermediate species acetylene (C_2H_2) in thermal radiation has not been considered in the numerical simulations of ethylene flames, which may lead to errors in the predictions of soot formation. Guo et al. [13] studied the fuel preheating effect on soot formation and considered the radiative heat transfer of soot, H_2O , CO_2 and CO in two-dimensional coflow ethylene laminar diffusion flames. The results showed that the maximal C_2H_2 and C_2H_4 mole fractions were 0.084 and 1.0, respectively, while the maximal CO mole fraction was 0.088, indicating that the radiation absorption of C_2H_2 and C_2H_4 cannot be ignored. In recent years, several studies on [14–16] the radiation absorption effect of hydrocarbon fuels in combustion have been performed. De Ris [17] first pointed out that the effect of radiative heat transfer from combustion products to the fuel surfaces exceeded the conductive heat transfer in pool fires. To quantify the radiation absorption effect of fuel on determining the mass consumption rate in pool fires, Brosmer et al. [18] proposed a two-region flame model to predict the radiative flame feedback. However, detailed spectrally resolved radiation absorption properties for

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hydrocarbon fuels were missing in these studies.

To obtain the radiative characteristics of gases, the most straightforward way is the line-by-line (LBL) method [16], which however, requires numerous spectral line data and excessive computation time. In order to get higher computational efficiency, Chu [19] proposed the Planck mean absorption coefficients method for H_2O , CO_2 , CO and CH_4 based on the LBL. This method does not need to solve the RTE but can be only used in optically thin cases. Since the radiative contribution of the mean absorption coefficient varies with the wavenumber, the narrow band models with low spectral resolution were proposed, such as the statistical narrow band (SNB) model [20–22], the spectral-line moment-based (SLMB) model [23] and the exponential wide-band (EWB) model. Soufiani et al. [24] generated narrow band (NB) parameters for H_2O , CO_2 and CO with a 25 cm^{-1} spectral resolution based on the HITEMP-2010 and CDSD-1000. To study pool fire radiation feedback, Consalvi et al. [25] established NB parameters for nine fuels (methane, methanol, ethane, ethylene, propane, propylene, heptane, methyl methacrylate and toluene) based on the NIST database. However, the narrow band models can be only used to obtain the gas transmissivity, which is suitable for solving the RTE in integral forms rather than differential forms. k -distribution methods can be used to obtain the gas absorption coefficient and are suitable for any RTE solver. Despite these previous studies, the k -distribution model for C_2H_2 and C_2H_4 , and the radiation effect of hydrocarbon fuels in the soot formation have never been investigated.

The goal of this study was to numerically investigate the radiation effects of C_2H_2 and C_2H_4 on the soot formation in a laminar coflow ethylene/air diffusion flame at atmospheric pressure. First, the SNBCK model parameters for C_2H_2 and C_2H_4 were generated based on the HITRAN 2016 database. Subsequently, temperature, soot volumetric fraction, radiative source and soot growth rate distributions at four different cases when considering the radiation effects of C_2H_2 and C_2H_4 were evaluated and discussed. Finally, the simulation results were compared with experimental data.

2. Numerical model and validation

The flame code used in this study has been documented by Zhang [26] and described in details in several previous studies [27–29]. The Navier-Stokes equations and transport equations for low Mach numbers are solved in a 2D axisymmetric domain to obtain the distributions of mass, momentum, energy, gas-phase component, soot mass fraction and number density. The equations are discretized and solved using the control volume method, and the pressure-velocity coupling is treated by the SIMPLE algorithm. The chemical reaction mechanism (101 species and 544 reactions) of Appel et al. [30] was used. The soot model employed in this study has been described in detail by Zhang et al. [31]. Soot inception is assumed to be a result of the collision of two pyrene molecules (A4). Surface growth and oxidation are assumed to follow the HACA mechanism [30]. All parameters associated with the HACA mechanism are taken from [30] and the fraction of the reactive soot surface sites $\alpha = 0.004\exp(10800/T)$ [32] is adopted in this study. The aggregation process of soot particles is modeled using a sectional aerosol dynamics model [31]. The sectional transport equations for soot aggregates and primary particles can be found in [31]. Soot nucleation rate is calculated by the collision rate of two pyrene molecules in the free-molecular regime, but enhanced by a factor of 2.2 due to van der Waals force [33]. PAH condensation on soot particles also contributes to the surface growth of soot. The radiative source in the energy conservation equation was solved by the discrete ordinates method (DOM) coupled with the SNBCK model for considering the radiative properties of H_2O , CO_2 , CO , C_2H_2 and C_2H_4 . The soot absorption coefficient $5.5f_p/\lambda$ developed by Hottel and Sarofim [34] based on the Rayleigh's theory and the refractive index of soot was used.

In the SNBCK model, the mean gas transmissivity in the SNB model can be expressed as the distribution function of the absorption

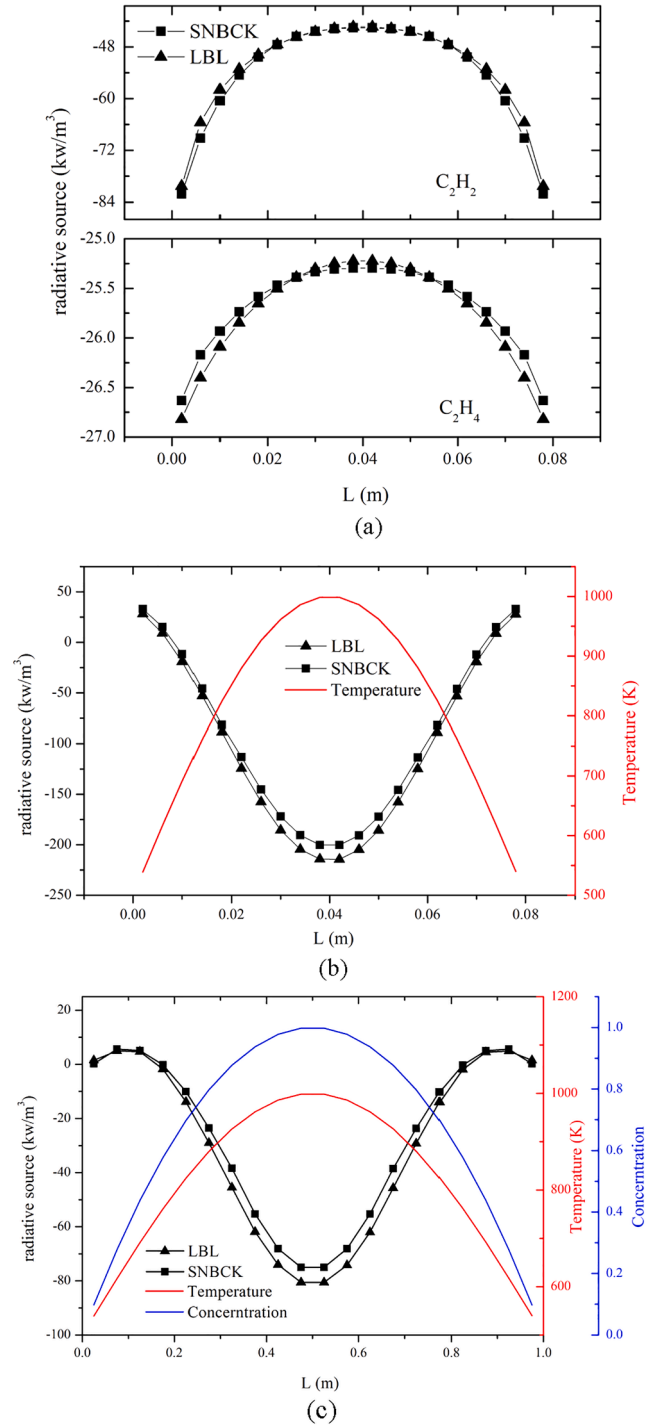


Fig. 1. Comparisons of radiative source calculated by SNBCK and LBL models for (a) $X_{C_2H_2} = 0.5$ at 1000 K in Case 1 and $X_{C_2H_4} = 0.5$ at 1000 K in Case 2; (b) a non-isothermal homogeneous gas mixture with temperature profile $500[1 + \sin(\pi x/L)]$ K, $X_{H_2O} = 0.1$, $X_{CO_2} = 0.1$, $X_{CO} = 0.05$, $X_{C_2H_2} = 0.05$ and $X_{C_2H_4} = 0.5$ in Case 3; (c) a non-isothermal inhomogeneous gas mixture with temperature profile $500[1 + \sin(\pi x/L)]$ K, $X_{H_2O} = X_{C_2H_2} = X_{C_2H_4} = 4(1-x/L) \times x/L$ in Case 4.

coefficient $f(k)$ in the narrow band through Laplace transform. With the Malkmus statistical narrow band model, the $f(k)$ can be described as [35]:

$$f(k) = \frac{1}{2} k^{-3/2} (BS)^{1/2} \exp \left[\frac{\pi B}{4} \left(2 - \frac{S}{k} - \frac{k}{S} \right) \right] \quad (1)$$

Table 1

Flow conditions (unit L/min) of the ethylene laminar diffusion flames at air atmosphere.

| Case | Air | Additional O ₂ | C ₂ H ₄ | O ₂ volume fraction |
|------|------|---------------------------|-------------------------------|--------------------------------|
| 1 | 240 | – | 0.194 | 0.21 |
| 2 | 240 | – | 0.150 | 0.21 |
| 3 | 75.9 | 44.1 | 0.194 | 0.5 |
| 4 | 91.1 | 28.9 | 0.194 | 0.4 |

where $B = 2\bar{\beta}_\eta/\pi^2$, $S = \bar{k}_\eta XP$ and $\bar{\beta}_\eta = 2\pi\bar{\gamma}_\eta/\bar{\delta}_\eta$. The SNB spectral parameters $\bar{\gamma}_\eta$, $\bar{\delta}_\eta$ and \bar{k}_η for H₂O, CO₂ and CO developed by Soufiani [24] were used. The spectral range in this work is from 150 to 9300 cm⁻¹ and the narrow bandwidth $\Delta\eta = 25$ cm⁻¹. The spectral line parameters for C₂H₂ and C₂H₄ are provided by HITRAN 2016. The narrow-band transmissivities of C₂H₂ and C₂H₄ calculated using the SNB and LBL models have been validated in Ref. [20]. C₂H₂ absorbs and emits radiation at all of the 367 narrow-bands while C₂H₄ has 52 radiating bands in the following two spectral regions: 675–1550 cm⁻¹ (36 bands) and, 2900–3275 cm⁻¹ (16 bands).

By introducing a cumulative function $g(k) = \int_0^k f(k')dk'$, Eq. (1) can be transformed to

$$g(k) = \frac{1}{2} \left[1 - \operatorname{erf}\left(\frac{a}{\sqrt{k}} - b\sqrt{k}\right) \right] + \frac{1}{2} \left[1 - \operatorname{erf}\left(\frac{a}{\sqrt{k}} + b\sqrt{k}\right) \right] e^{\pi B} \quad (2)$$

where $a = \sqrt{\pi BS}/2$, $b = \sqrt{\pi B/S}/2$ and $\operatorname{erf}(x)$ is the error function $\operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt$. For each Gauss-Lobatto quadrature point g_i , the corresponding absorption coefficient $k_i = k(g_i)_\eta$ can be calculated iteratively by solving Eq. (2) using a combined Newton-Raphson and bisection method [36].

After getting the absorption coefficients of H₂O, CO₂, CO, C₂H₂, C₂H₄ and soot, the RTE can be solved by DOM. The discrete ordinates form of the RTE in a cylindrical coordinate system is [37]:

$$\frac{\mu_{m,l}}{r} \frac{\partial r I_{m,l}}{\partial r} - \frac{1}{r} \frac{\alpha_{m,l+1/2} I_{m,l+1/2} - \alpha_{m,l-1/2} I_{m,l-1/2}}{\omega_{m,l}} + \xi_{m,l} \frac{\partial I_{m,l}}{\partial z} = -k_{g(i)} (I_B - I_{m,l}) \quad (3)$$

where m is the polar angle, l the azimuth angle and, $\omega_{m,l}$ the quadrature weight.

Once the intensity field is calculated, the radiative source of each volume can be expressed as:

$$\nabla \cdot \mathbf{q} = \sum_{i=1}^N w_i k_{g(i)} \left(4\pi I_B - \sum_{m=1}^M \sum_{l=1}^{L(m)} \omega_{m,l} I_{m,l} \right) \quad (4)$$

where N is the Gauss points and w_i the corresponding weight factor.

Model validations were conducted in four representative cases to assess the accuracy of the SNBCK model in predicting the absorption coefficients of C₂H₂ and C₂H₄. The thermal radiation heat transfer in a

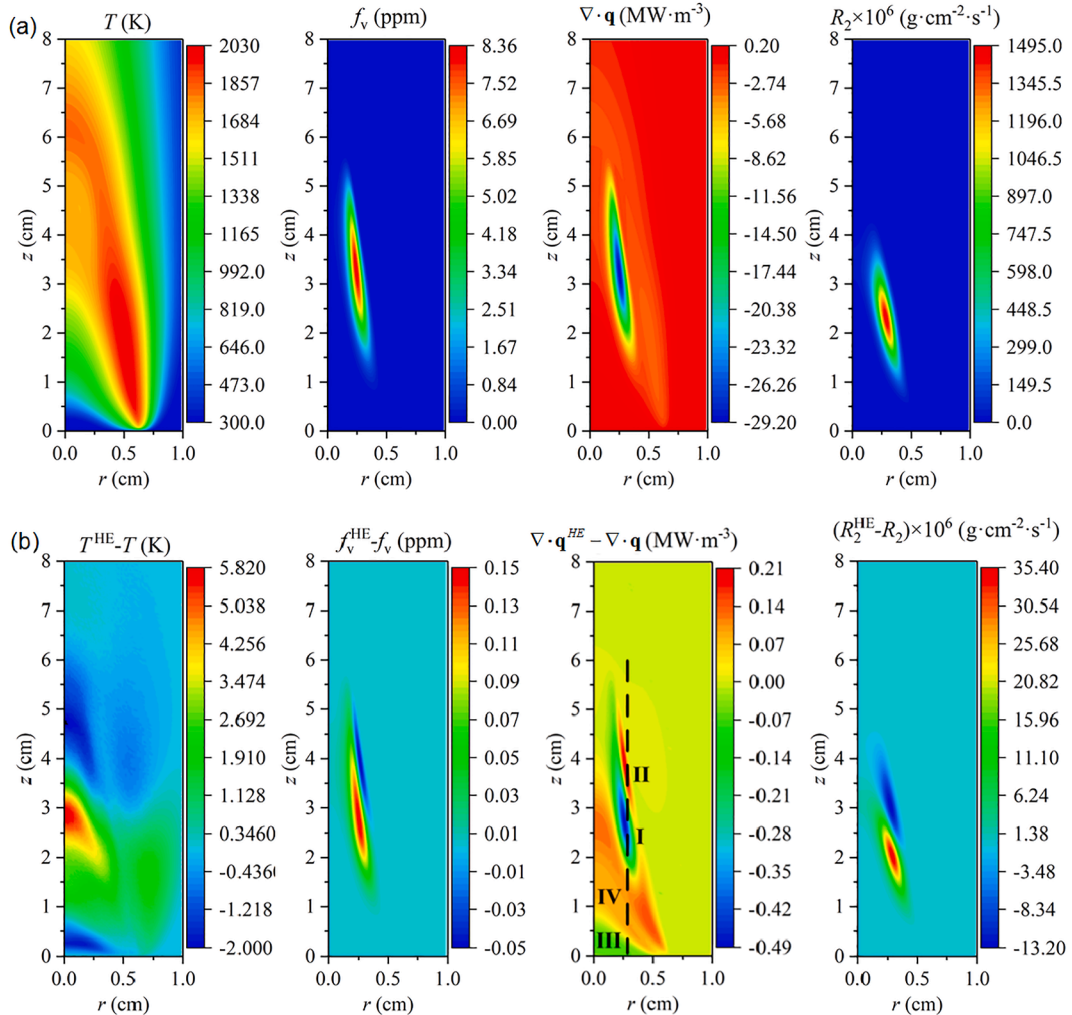


Fig. 2. (a) Distributions of the temperature T , soot volume fraction f_v , radiative source $\nabla \cdot \mathbf{q}$ and soot growth rate R_2 of Case 1; (b) distribution differences caused by the C₂H₂/C₂H₄ radiation effects in Case 1. Superscript HE denotes hydrocarbons excluded (i.e. without C₂H₂ and C₂H₄ radiation).

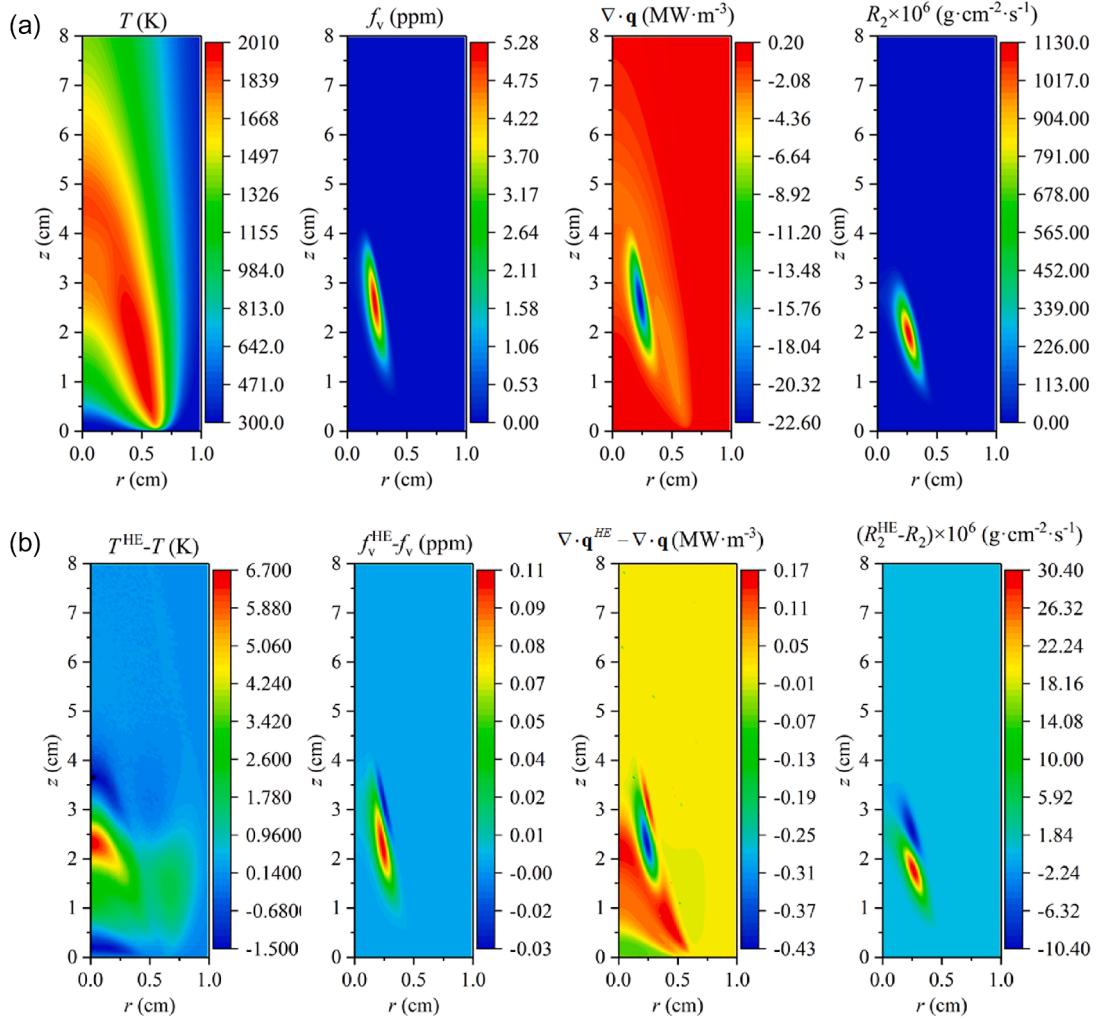


Fig. 3. (a) Distributions of the temperature T , soot volume fraction f_v , radiative source $\nabla \cdot \mathbf{q}$ and soot growth rate R_2 of Case 2; (b) distribution differences caused by the $\text{C}_2\text{H}_2/\text{C}_2\text{H}_4$ radiation effects in Case 2. Superscript HE denotes hydrocarbons excluded (i.e. without C_2H_2 and C_2H_4 radiation).

one-dimensional planar slab was investigated and total pressure was fixed as 1 atm. These four cases contained an isothermal and homogeneous medium, non-isothermal homogeneous medium and non-isothermal inhomogeneous medium: $X_{\text{C}_2\text{H}_2} = 0.5$ at 1000 K in Case 1, $X_{\text{C}_2\text{H}_4} = 0.5$ at 1000 K in Case 2, the temperature of $500[1 + \sin(\pi x/L)]$ K, $X_{\text{H}_2\text{O}} = 0.1$, $X_{\text{CO}_2} = 0.1$, $X_{\text{CO}} = 0.05$, $X_{\text{C}_2\text{H}_2} = 0.05$ and $X_{\text{C}_2\text{H}_4} = 0.5$ in Case 3, the temperature of $500[1 + \sin(\pi x/L)]$ K, $X_{\text{H}_2\text{O}} = X_{\text{C}_2\text{H}_2} = X_{\text{C}_2\text{H}_4} = 4(1-x/L) \times x/L$ in Case 4. The two slabs were diffusive black body with temperature 300 K. The parallel-plane space were segmented into 20 uniform volumes. As shown in Fig. 1, the comparisons between the LBL and SNBCK results show favorable agreements, illustrating the quality of the applied model parameter adjustments.

3. Results and discussion

Coflow laminar diffusion flames have been established by Gülder's burner [38] and were modeled in [27,32,39]. The fuel stream passes through the 10.9 mm inner diameter tube, while the air flow goes through an annular having the outer diameter of 88.7 mm. A non-uniform mesh with 332×87 control volumes (in the flow direction z and radial direction r , respectively) for the $15.353 \times 6.0 \text{ cm}^2$ channel domain yielded grid-independent solutions. At the nozzle, the radial mesh length is 0.069 mm and the axial mesh length is 0.125 mm. The flow conditions of the four cases studied are summarized in Table 1. In Cases 1 and 2 air was used in the oxidizer flow, while Cases 3 and 4 had

additional O_2 in air, i.e. "rich-oxygen conditions".

Fig. 2(a) shows the temperature, soot volumetric fraction, radiative source and soot growth rate distributions when considering the radiation effects of C_2H_2 and C_2H_4 . The peak flame temperature was located in the annular region near the flame flank $r = 0.5 \text{ cm}$, $z = 1\text{--}3 \text{ cm}$, and the flame front was closed near the $z = 6 \text{ cm}$. The peak soot volume fraction was located at $r = 0.25 \text{ cm}$, $z = 2\text{--}4 \text{ cm}$, since the soot is easy to generate at the fuel-enriched and high temperature region. The radiative source was affected by both distributions of temperature and soot volumetric fraction. The radiative source at the high soot volumetric fraction region is larger than that at the high temperature region, due to the stronger radiation capacity of soot than that of gaseous species. The soot growth rate distribution was similar to the acetylene concentration distribution (see Fig. 10 in [13]), except in the area near the axis where the soot growth rate is low caused by the less soot nucleation and lower temperature.

To facilitate discussions on the radiation effects of C_2H_2 and C_2H_4 in Fig. 2(b), the whole domain was categorized into four regimes based on the radiative source distributions: Regime I, $\nabla \cdot \mathbf{q} < 0$, $\nabla \cdot \mathbf{q}^{\text{HE}} - \nabla \cdot \mathbf{q} < 0$ (radiative heat emission, the heat emission value decreased when considering the $\text{C}_2\text{H}_2/\text{C}_2\text{H}_4$ radiation); Regime II, $\nabla \cdot \mathbf{q} < 0$, $\nabla \cdot \mathbf{q}^{\text{HE}} - \nabla \cdot \mathbf{q} > 0$ (radiative heat emission, the heat emission value increased when considering the $\text{C}_2\text{H}_2/\text{C}_2\text{H}_4$ radiation); Regime III, $\nabla \cdot \mathbf{q} > 0$, $\nabla \cdot \mathbf{q}^{\text{HE}} - \nabla \cdot \mathbf{q} < 0$ (radiative heat absorption, the heat absorption value increased when considering the $\text{C}_2\text{H}_2/\text{C}_2\text{H}_4$ radiation); Regime IV,

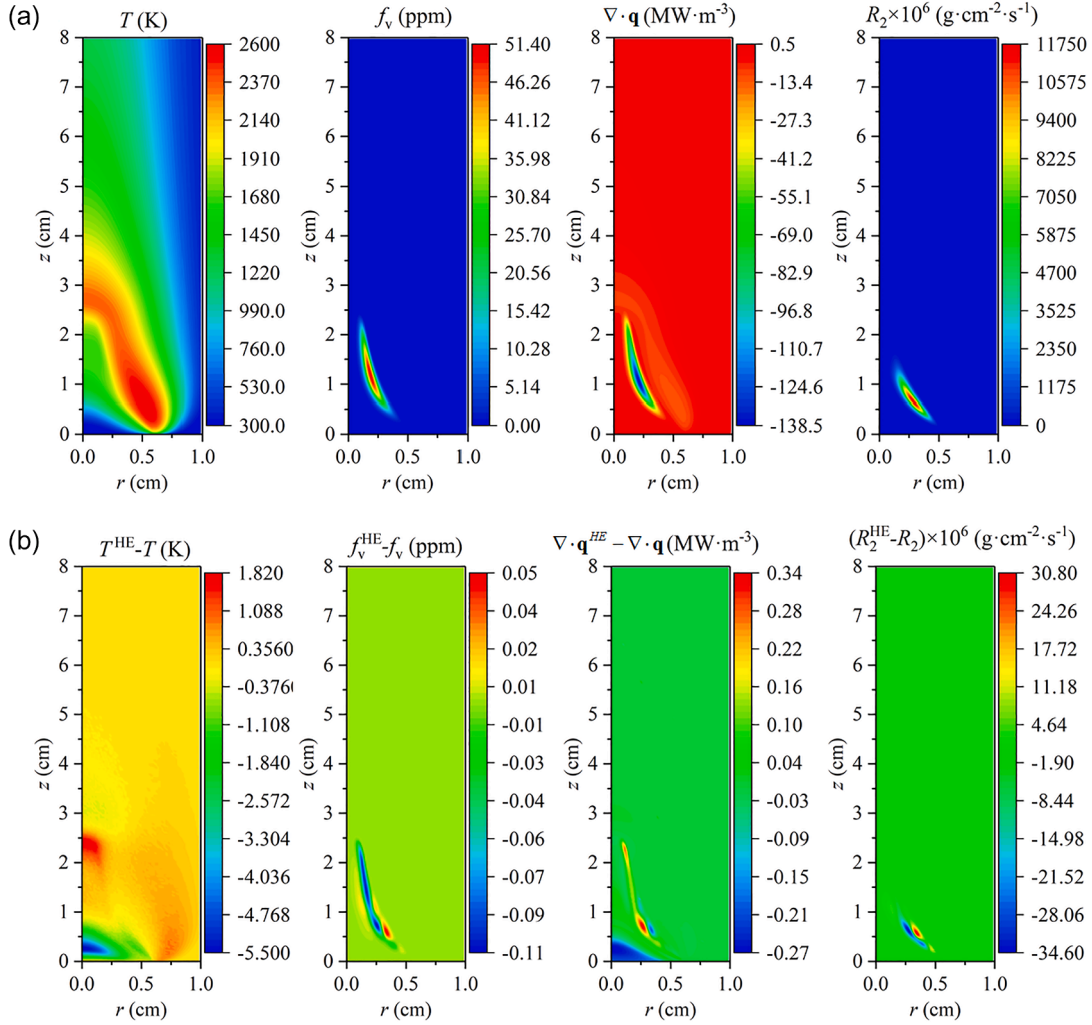


Fig. 4. (a) Distributions of the temperature T , soot volume fraction f_v , radiative source $\nabla \cdot q$ and soot growth rate R_2 of Case 3; (b) distribution differences caused by the C_2H_2/C_2H_4 radiation effects in Case 3.

$\nabla \cdot q > 0$, $\nabla \cdot q^{HE} - \nabla \cdot q > 0$ (radiative heat absorption, the heat absorption value decreased when considering the C_2H_2/C_2H_4 radiation).

As shown in Fig. 2(b), along the flow direction the radiative source $\nabla \cdot q$ in the burner outlet fell in Regime III. The predicted flame temperature decreased when the effects of C_2H_2/C_2H_4 radiation was absent due to fact that the high C_2H_4 concentration near the burner outlet absorbed radiation energy from the downstream burning area of the flame. Along the streamwise direction, Regime IV was realized downstream to Regime III. The reason is that the gas radiative emission energy increased with the rising C_2H_2 concentration and flame temperature. Subsequently, further downstream location along the dashed line fell in Regime I, where the flame temperature decreased when considering the effects of C_2H_2/C_2H_4 radiation due to the radiative heat loss to upstream locations of Regimes III and IV. As a result, the local soot formation was delayed and the radiative source decreased significantly at the same location in the presence of realistic C_2H_2/C_2H_4 radiation. Regime II was finally reached at the most downstream locations, where the radiative emission energy increased due to the delayed soot formation. This is also supported by the distributions of soot volumetric fraction f_v and soot growth rate R_2 .

As shown in Fig. 3, Case 2 exhibited qualitatively similar distributions of gas temperature, soot volumetric fraction, radiative source and soot growth rate as Case 1. As the fuel flow rate of Case 2 was less than that of Case 1, the peak gas temperature and soot volumetric fraction in Case 2 were lower than those in Case 1. The maximum value of soot

volumetric fraction is shown to move downward and inward in the spatial distribution caused by the reduced fuel flow rate.

To delineate the C_2H_2/C_2H_4 radiation effects at higher soot volumetric fraction, oxygen concentration in the oxidizer flows in Case 3 was increased by introducing additional O_2 in the air stream. As shown in Fig. 4(a), comparing to the Cases 1 and 2, the height of the flame decreased, while the soot was only distributed below 25 mm.

Fig. 4(b) shows that the flame temperature near the nozzle outlet was higher than that without considering the C_2H_2/C_2H_4 radiation effect. This difference was larger than in Case 1 due to its higher peak gas temperature and soot volume fraction. The difference of soot growth rate indicates that soot was more likely to form near the axis of symmetry ($r = 0$) when considering the C_2H_2/C_2H_4 radiation effect comparing to Cases 1 and 2. The reason was that the soot precursor concentration near the nozzle increased with the rising radiative absorption. Compared with Cases 1 and 2, the peak of radiative source difference ($\nabla \cdot q^{HE} - \nabla \cdot q$) moved from the high soot volumetric fraction region ($z \sim 2.5$ cm, see Fig. 2(b) and 3(b)) to the high C_2H_4 concentration region near the nozzle outlet. Moreover, the area of $\nabla \cdot q^{HE} - \nabla \cdot q > 0$ was larger than that of $\nabla \cdot q^{HE} - \nabla \cdot q < 0$ in Case 3 which was the opposite to Case 1 and 2, indicating stronger emission and weaker absorption. The reason was that the peak soot volumetric fraction increased when considering the C_2H_2/C_2H_4 radiation effect in the oxygen-enriched case.

Qualitatively similar to those of Case 3 but quantitatively lower

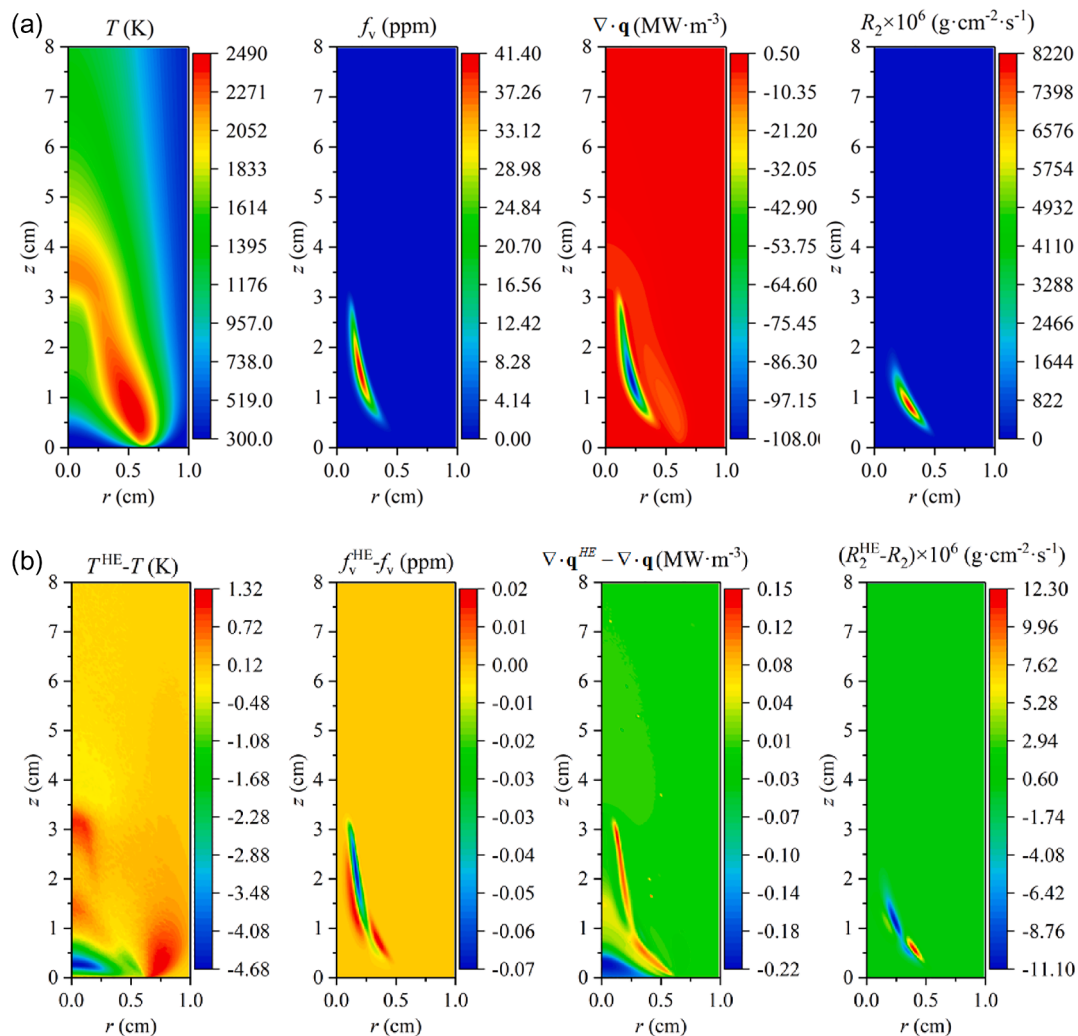


Fig. 5. (a) Distributions of the temperature T , soot volume fraction f_v , radiative source $\nabla \cdot \mathbf{q}$ and soot growth rate R_2 of Case 4; (b) distribution differences caused by the $\text{C}_2\text{H}_2/\text{C}_2\text{H}_4$ radiation effects in Case 4. Superscript HE denotes hydrocarbons excluded (i.e. without C_2H_2 and C_2H_4 radiation).

temperatures and soot volumetric fraction distributions were obtained in Case 4 as shown in Fig. 5, due to the decreased oxygen addition into the air flow.

To quantitative analysis the $\text{C}_2\text{H}_2/\text{C}_2\text{H}_4$ radiation effect on the soot volume fraction, the relative changes of the soot volume fraction ($f_v^{\text{HE}} - f_v$)/ f_v at main soot formation heights ($z = 2.0, 2.5$ and 3.0 cm for Case 1 and 2, $z = 0.8, 1.0$ and 1.2 cm for Case 3 and 4) were shown in Fig. 6. For Case 1 and 2, the maximum radiation effect was 9% at $z = 2.5$ cm and 9.46% at $z = 2.0$ cm, respectively. In the Fig. 6(a) and (b), the radiation effect showed positive first and then negative. For Case 3 and 4, the maximum radiation effect was 5.7% at $z = 0.8$ cm and 9.87% at $z = 0.8$ cm, respectively. In the Fig. 6(c) and (d), the radiation effect trend showed different from the Fig. 6(a) and (b), decreased first and then increased. The reason was that the soot formation was easier to happen near the axis of symmetry for oxygen-enriched cases which shown in Figs. 4 and 5.

However, the height corresponding to the maximum soot volumetric fraction was significantly affected by the radiation from C_2H_2 and C_2H_4 , as summarized in Table 2. When the $\text{C}_2\text{H}_2/\text{C}_2\text{H}_4$ radiation effect was considered in the simulations, the height $Z_{\text{max}(f_v)}$ corresponding to the maximum soot volumetric fraction increased by 3.04% and 1.88% in Cases 1 and 2, respectively. The reason was that the soot formation was delayed towards to the downstream direction and the overlapping region of soot formation and oxidation was enlarged by the effects of $\text{C}_2\text{H}_2/\text{C}_2\text{H}_4$ radiation. For Cases 3 and 4 at oxygen-enriched conditions,

the height $Z_{\text{max}(f_v)}$ corresponding to the maximum soot volumetric fraction decreased by 7.49% and 5.73%, respectively. This was caused by the change of temperature distribution, which moved the radial position of soot formation towards the axis of symmetry where C_2H_2 concentration was higher.

The calculated soot volumetric fractions considering the $\text{C}_2\text{H}_2/\text{C}_2\text{H}_4$ radiation effect and no $\text{C}_2\text{H}_2/\text{C}_2\text{H}_4$ radiation effect in Case 1 were compared to the experimental measurements reported by Liu et al. [40] and Snelling et al. [41]. The soot volume fractions measured by two-dimensional line-of-sight light attenuation (LOSA) corrected for scatter [41] were compared in Fig. 7.

Radial profiles of f_v at two selected heights are shown in Fig. 7. Experimental data was discarded at $r < 1.5$ mm due to the large measurement noise. It can be seen that the simulations considering the $\text{C}_2\text{H}_2/\text{C}_2\text{H}_4$ radiation effect well reproduced the profiles, especially the locations and peak values of soot volumetric fraction. When considering the $\text{C}_2\text{H}_2/\text{C}_2\text{H}_4$ radiation effect, the average relative errors were 13.4%, 12.1% and 25.4% at $z = 2$ cm, $z = 3$ cm and 4 cm. However, the average relative errors were 23.8%, 13.3% and 31.1% at $z = 2$ cm, $z = 3$ cm and 4 cm for no $\text{C}_2\text{H}_2/\text{C}_2\text{H}_4$ radiation effect. Therefore, the simulation results were improved by 10.4% at $z = 2$ cm in the flame of Case 1 when considering the $\text{C}_2\text{H}_2/\text{C}_2\text{H}_4$ radiation.

Apart from the dominating oxidative pyrolysis in non-premixed jet flames, other important reactions affecting C_2H_2 concentration were finally identified via the sensitivity analysis (SA) in a homogeneous

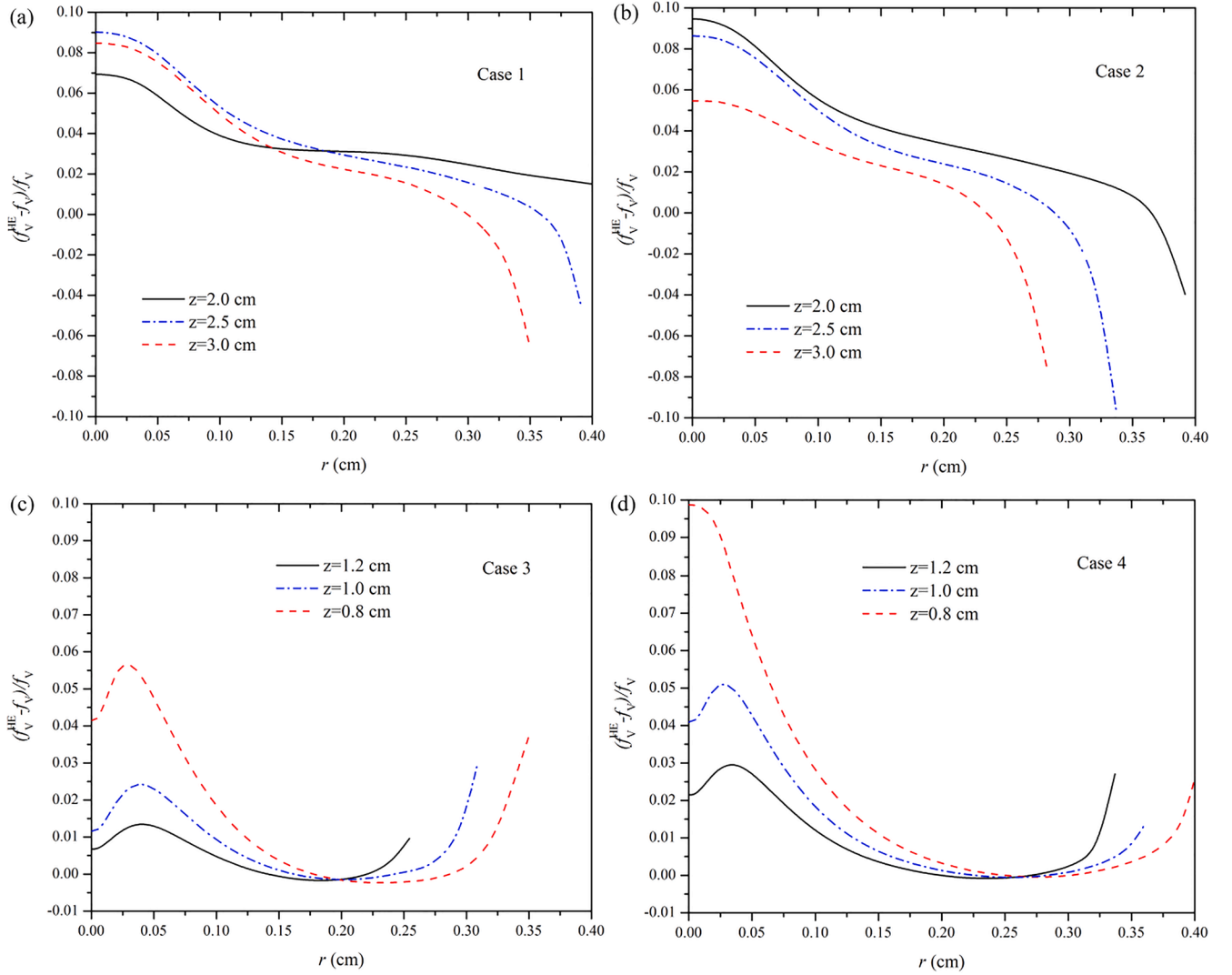


Fig. 6. C_2H_2/C_2H_4 radiation effect on the soot volume fraction (a) Case 1; (b) Case 2; (c) Case 3; (d) Case 4.

Table 2

The C_2H_2/C_2H_4 radiation effect on the height $Z_{\max}(f_v)$ corresponding to the maximum soot volumetric fraction.

| Case | 1 | 2 | 3 | 4 |
|--------------------------------------|--------|--------|-------|-------|
| $Z_{\max}(f_v)$ (cm) | 3.29 | 2.60 | 1.17 | 1.51 |
| $Z_{\max}(f_v)^{HE}/Z_{\max}(f_v)-1$ | -3.04% | -1.88% | 7.49% | 5.73% |

system as shown in Fig. 8. The two controlling reactions were C_2H_2 reactions with O radical, i.e. $C_2H_2 + O = CH_2 + CO$ and $C_2H_2 + O = HCCO + H$ with negative sensitivity coefficients and $C_2H_4 + OH = C_2H_3 + H_2O$ with a positive sensitivity coefficient. Therefore, the consumption of C_2H_2 is mainly dominated by the availability of O while OH plays an important role in C_2H_2 formation.

4. Conclusions

A numerical study was conducted to investigate the radiation effects of C_2H_2 and C_2H_4 on soot formation in a laminar coflow ethylene/air diffusion flame at atmospheric pressure. The SNBCK model parameters for C_2H_2 and C_2H_4 were generated from SNB calculations based on the HITRAN 2016 database and were validated by the LBL method. The simulations well reproduced the literature experimental data of soot

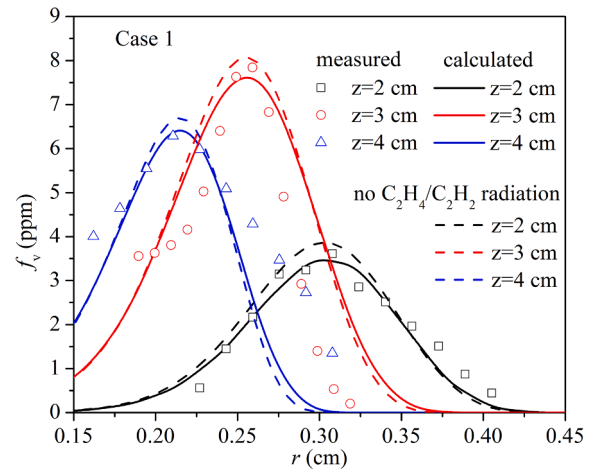


Fig. 7. Soot volumetric fraction f_v profiles as a function of radial location in the flame of Case 1 at height of 2 cm and 4 cm compared with hyperspectral imaging results in [40] and the height of 3 cm compared with two-dimensional LOSA scatter-corrected soot volume fractions in [41].

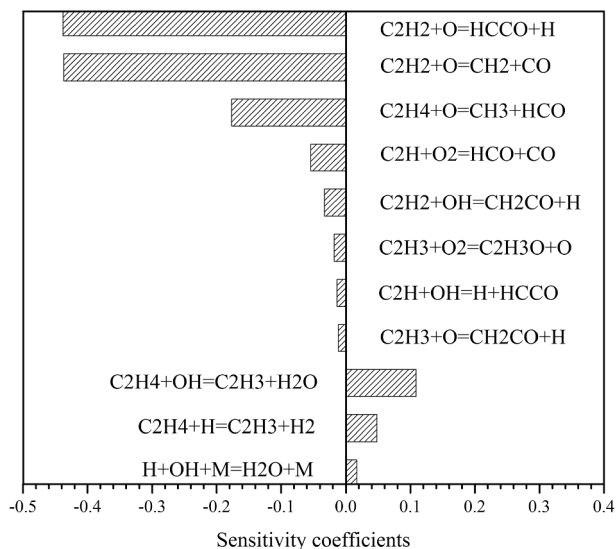


Fig. 8. Sensitivity coefficients of C_2H_2 concentration in a perfectly stirred reactor for C_2H_4 /air flame.

volumetric fraction. The present results revealed that the position of soot formation was affected by the temperature distribution when considering the C_2H_2/C_2H_4 radiation, due to the radiation absorption of C_2H_4 at low temperatures and the radiation emission of C_2H_2 at high temperatures. When considering the C_2H_2/C_2H_4 radiation, for air conditions the height corresponding to the maximum soot volumetric fraction increased because the overlapping region of soot formation and oxidation was enlarged, while for oxygen-enriched conditions the height corresponding to the maximum soot volumetric fraction decreased as a result of soot formation shift towards the axis of symmetry where C_2H_2 concentration was higher. C_2H_2 concentration was mainly dominated by radical O and OH radicals as revealed by sensitivity analyses.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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