Numerical Investigations on Methane–Air Nanosecond Pulsed Dielectric Barrier Discharge Plasma-Assisted Combustion

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ABSTRACT: Plasma-assisted combustion is a promising approach to achieve fast ignition and highly efficient combustion. In this work, methane–air nanosecond pulsed dielectric barrier discharge plasma-assisted combustion is numerically investigated by combining a homemade plasma model with the combustion model of software CHEMKIN-PRO. Effects of varying applied voltage amplitudes on the characteristic parameters of the plasma-assisted planar shear flow combustion as well as the reaction pathway maps of not only the nanosecond pulsed dielectric barrier discharge plasma but also the combustions without and with plasma assistance are systematically illustrated and analyzed. The simulation results indicate that under the combined action of increasing electric field intensity and increasing charged particle densities, the peak value of the discharge current density increases, and the peak time of the discharge current density is brought forward with the increase of the applied voltage amplitude. The temperature reaches its peak value earlier in the methane–air combustion with plasma assistance than without plasma assistance. The maximum temperature reduces to around 1900 K when the applied voltage amplitude is higher than 11 kV. There are emerging pathways to generate hydrocarbons C2H4 and C2H2 in the plasma-assisted combustion, the reactions of CH4 on CH and C2H on H2, respectively. The reactions involving active species such as H play a significant role in the plasma-assisted combustion, which causes an obvious decrease in the densities of these active species with plasma assistance.

1. INTRODUCTION

Methane is extensively used in domestic and industrial applications such as combustion, generation of electric power, and hydrogen production by partial oxidation. Methane combustion not only supplies energy and power to human society but also emits toxic byproducts that have harmful effects on the environment. Emerging methane combustion techniques including catalytic combustion and plasma-assisted combustion can reduce the combustion temperature and the pollutant emission, and hence, have become highly appealing combustion ways, thereby attracting attention of researchers.

The discharge plasma provides a promising process to realize fuel decomposition and conversion as well as gas purification and abatement, and thus it has been utilized to assist ignition and flame stabilization. The major enhancement effects of the discharge plasma-assisted combustion have been regarded as the thermal enhancement effect, the kinetic enhancement effect, and the transport enhancement effect. As far as the kinetic enhancement effect is concerned, the radicals formed in the plasma react with the fuel, resulting in chain-branching reactions and heat generation, which can eventually help in enhancing combustion. In comparison with equilibrium discharge plasmas, i.e., spark discharge plasma and arc discharge plasma, nonequilibrium discharge plasmas such as nanosecond pulsed discharge (NPD) plasma, dielectric barrier discharge (DBD) plasma, and nanosecond pulsed DBD (NPDBD) plasma could generate abundant high-energy electrons and radicals, forming the remarkable kinetic enhancement effect to effectively assist the fossil fuel combustion.

Aleksandrov et al. simulated the ignition dynamics of the methane–air plasma. It has been found that the NPD plasma produces active species, i.e., oxygen atoms, causing accelerations of chain reactions and ignition processes. Deminskii et al. studied influences of electronically excited species and vibrationally excited species on the NPD plasma-assisted combustion of methane–air and hydrogen–air in the initial temperature range of 500–900 K. It has been shown that the quenching of electronically excited nitrogen leads to the dissociation of the methane molecule at the early stage of combustion. Vincent-Randonnier et al. established a coaxial DBD burner that has a metallic needle located at the axis of the shell and is connected to the alternating current high-voltage power supply. It has been found that the DBD plasma can affect the flame structure and reduce the flame detachment...
height. De Giorgi et al. investigated the effects of the DBD plasma on methane decomposition for the combustion enhancement of the lean flame. It has been shown that the gas temperature increases by 294.8 K and the fuel composition is slightly modified under the assistance of the DBD plasma.

The NPDBD plasma combines the advantages of the NPD plasma and the DBD plasma, and therefore, is considered as the suitable nonequilibrium discharge plasma for assisting combustion. Lefkowitz et al. set up an experimental platform for 8.3% CH₄, 16.7% O₂, and 75% He at a temperature of 407 K and a pressure of 60 Torr and studied the temperature increase and the reaction path of fuel consumption in a single pulse period of the NPDBD plasma. Takana et al. developed the two-dimensional numerical simulation of the methane–air NPDBD plasma with a high energy loading for typical conditions of internal engines. Though the NPDBD plasma-assisted combustion has been experimentally and numerically investigated over the past decade, research studies on influences of the changing applied voltage on the characteristics of the DBD plasma-assisted combustion derived by nanosecond pulsed voltage at atmospheric pressure are still less reported. Spatial-temporal evolutions and reaction pathways of the NPDBD plasma and the corresponding plasma-assisted combustion in methane–air mixtures under different applied voltages should be further studied and illustrated.

In this work, a homemade plasma model and a combustion model based on software CHEMKIN-PRO have been used to numerically study the methanear air NPDBD plasma-assisted planar shear flow combustion. The purpose of this work is to explore the influences of varied applied voltage amplitudes on characteristic parameters of the plasma-assisted combustion. In addition, the reaction pathway maps of not only the NPDBD plasma but also the planar shear flow combustions without and with plasma assistance have been presented and analyzed. The rest of this manuscript is organized as follows. Effects of varying the applied voltage amplitude on discharge current densities and particle densities of the methane–air plasma are presented and discussed in Section 2.1. Combustion temperatures and particle mole fractions of the methane–air planar shear flow combustion under different applied voltage amplitudes are illustrated in Section 2.2. Reaction pathway maps of the NPDBD plasma and the combustions without and with plasma assistance are shown in Section 2.3. Conclusions are summarized in Section 3. The plasma model and the combustion model are introduced in Sections 4.1 and 4.2, respectively.

2. RESULTS AND DISCUSSION

2.1. Effects of Varying the Applied Voltage Amplitude on the Methane–Air NPDBD Plasma. Figure 1 presents the simulation results of the applied voltage $V_a$, the discharge gap voltage $V_g$, and the discharge current density $I_g$ calculated by the present methane–air NPDBD plasma model under a methane equivalent ratio of 0.9. Figure 2 shows the experimental results of $V_a$ and $I_g$ derived from the methane–air NPDBD plasma experiment in ref 28. Although the pulse parameters of the applied voltage and other discharge conditions in the simulation are not completely identical with those in the experiment, similar discharge current density waveforms in the two figures should illustrate that the simulation results are in agreement with the experiment results. Figure 3 shows the discharge current densities in the methane–air NPDBD plasma under different amplitudes of the applied voltage. It can be seen that with the increase of the applied voltage amplitude, the maximum discharge current density increases and the moment when the discharge current density reaches the maximum occurs earlier. Figure 4 illustrates the averaged particle densities of the electrons, all negatively charged particles, all positively charged particles, and the maximum discharge current densities in the methane–air NPDBD plasma under different amplitudes of the applied voltage. The averaged particle density of a certain particle is the result of the sum of the particle numbers in the discharge region for one period of the applied pulsed voltage divided by both the volume of the discharge region and the period of the pulsed voltage. This figure indicates that the averaged particle densities and the maximum discharge current density obviously increase with the increase of the applied voltage.
amplitude in the methane–air NPDBD plasma. The electric field directly affects the electron energy distribution function and then the excitation of the electron. The electron deposited electrical energy is faster in the higher electric field with increasing applied voltage amplitude, thereby accelerating the processes of electron collision ionization, dissociation, and electronical excitation. This generates more ions, free radicals, and electronically excited species, which makes the discharge to occur earlier.

Figure 5 helps to further understand the spatial characters of the NPDBD plasma. This figure gives the spatial distributions of the electric field intensities and densities of all negatively charged particles and all positively charged particles at the time when the discharge current density reaches the maximum in the methane–air NPDBD plasma under different amplitudes of the applied voltage. It can be seen that when the applied voltage amplitude is higher than 9 kV, there is a distinct cathode fall with the maximum electric field intensity value close to 80 kV/cm on the left side. In the region of the high electric field intensity, the densities of both all positively charged particles and all negatively charged particles reach the order of magnitude of $10^{13}$ cm$^{-3}$. The region of the high electric field intensity can be identified as the cathode sheath region of the NPDBD plasma. Except for the cathode sheath region, in other places of the discharge gap, the electric field intensities approximate to $10^{12}$ cm$^{-3}$. The region of the low electric field intensity can be regarded as the positive column region of the NPDBD plasma. Furthermore, in the discharge gap, not only the electric field intensities but also the charged particle densities increase with the increase of the applied voltage amplitude.

It is known that the discharge current density results from the movement of the charged particles, and therefore, under the combined action of the increasing electric field intensity and the increasing charged particle densities, the maximum discharge current density increases with the increase of the applied voltage amplitude, as shown in Figures 3 and 4. In addition, because the cathode sheath region and the positive column region are not formed in Figure 6, the applied voltage amplitude of 9 kV should be insufficient to activate the methane–air NPDBD plasma under the present discharge conditions.

The averaged particle densities of the significant active species in the methane–air NPDBD plasma under different amplitudes of the applied voltage are shown in Figure 6. This figure illustrates that the atom O is the active species having the highest particle density in the methane–air NPDBD plasma. Under different amplitudes of the applied voltage, the averaged particle densities of other active species are at least 1 order of magnitude lower than the averaged particle densities of the atom O. Hydroxyl OH and methyl CH$_3$ have similar
averaged particle densities, which are slightly lower than the averaged particle densities of the atom H. The above results are in agreement with the simulation results in ref 26.

2.2. Effects of Varying the Applied Voltage Amplitude on the Methane–Air NPDBD Plasma-Assisted Combustion. Figures 7 and 8 show the two-dimensional spatial evolutions of the temperatures and the mole fractions of CH₃ in the methane–air planar shear flow combustions without and with plasma assistance, respectively. It is shown that the effects of the NPDBD plasma on the radial characteristics of the planar shear flow combustion are not evident. The one-dimensional simulation results based on the averaged values in the radial direction are presented in the rest of Section 2.2.

The temperatures in the methane–air planar shear flow combustions without and with plasma assistance are shown in Figure 9. It can be seen that the temperature reaches its peak value earlier in the methane–air combustion with plasma assistance than that in without plasma assistance. Moreover, the maximum temperature has a value of around 2200 K when the applied voltage amplitude is 9 or 10 kV but has a value of around 1900 K when the applied voltage amplitude varies from 11 to 13 kV. With the increase of the applied voltage amplitude, the moment when the temperature reaches the maximum occurs on-going earlier, but there is little change in the maximum temperature when the applied voltage amplitudes changes from 11 to 13 kV. With the thermal energy from the burner wall, the chain-branching reactions cause a rapid increase in the concentration of the chain carrier and the reactant, resulting in a dramatic increase in the reaction rate around 190 cm forming the flame in the methane–air combustion without plasma assistance. When the discharge occurs, the active species are effectively generated in methane–air NPDBD plasma so as to accelerate the process of the chain-branching reactions by the kinetic effect, moving the flame upstream. Although 9 kV discharge is not sufficient to form the methane–air NPDBD plasma, it can assist methane–air combustion through produced radicals in the discharge. The maximum heat production rate hits 3 W/cm³ in methane–air combustion without plasma assistance, and it rises to 6.2 or 14 W/cm³ in methane–air combustion with plasma assistance with an applied voltage amplitude of 9 or 10 kV. As the applied voltage amplitude increases from 11 to 13 kV, the maximum heat production rate varies around 2 W/cm³.

Mole fractions of the major species in the methane–air combustion are plotted in Figures 10 and 11. When the applied voltage amplitude is not lower than 11 kV, the mole fractions of CH₃, HO₂, CH₂OH, C₂H₆, C₂H₅ and CH₂O are higher than those when the applied voltage amplitude is 9 or 10 kV, and the mole fractions of these particles increase with the increase of the applied voltage amplitude, which implies that the NPDBD plasma-assisted combustion could get the better performance, as the applied voltage amplitude is higher. Meanwhile, the mole fractions of O, H, and OH show a downward trend as the applied voltage amplitude increases.
from 11 to 13 kV, which means that the active species are more dramatically consumed in the combustion reactions under the higher applied voltage amplitude of the NPDBD plasma. As the applied voltage amplitude varies from 9 to 13 kV, the effects of the methane–air plasma on the atom O-consuming reactions in the combustion are complex. Reactions O + CH4 → OH + CH3 and O + CH2O → OH + HCO are the dominant atom O-consuming reactions in the methane–air combustion without and with plasma assistance. When the applied voltage amplitude is 9 or 10 kV, the reaction rate of O + CH2O → OH + HCO decreases. When the applied voltage amplitude varies from 11 to 13 kV, other reaction rates between O and H2, HO2, or H2O2 increase.

2.3. Reaction Pathway Maps of the Methane–Air NPDBD Plasma and the Methane–Air NPDBD Plasma-Assisted Combustion. Figure 12 displays the reaction pathways consuming various kinds of particles in the methane–air NPDBD plasma when the applied voltage amplitude is 11 kV. In this figure, the solid line and the dashed line stand for the primary reaction path (reaction contribution is higher than 10%) and the secondary reaction path (reaction contribution is not higher than 10%) to consume the species, respectively. Other species that participate in the reaction and the reaction contribution to consuming the species are shown in the middle of the line. Figure 12 indicates that 41.6% of the methane reacts with the electron or the excited species to form CH3. CH3 can also be generated by the consumption of CH and CH2. In total, 3.5 and 13.9% of the methane react with the neutral particles C and CH2 (or CH) to produce C2H2 and C2H4, respectively. The majority of N2 collides with the electron to produce the excited states N2(B) and N2(a′) and the atom N. In total, 88.5% of the atom N reacts with O2 or OH to form NO. Atom O can be formed by the reaction between the excited state species and the neutral species, i.e., N2(A) + O2 → N2 + O + O as well as the reaction between the two neutral species, i.e., N + NO → N2 + O.

The reaction pathway map of the methane–air combustion without plasma assistance is illustrated in Figure 13. The majority of methane reacts with OH, HO2, CH3, and O to form CH3. Of all, 78.1% of CH3 reacts with HO2 to produce CH3O, and then 97.5% of CH3O is consumed to generate CH2O. At the same time, 10.4% of CH3 is consumed to form C2H6, which is the origin to form hydrocarbons such as C2H5, C2H4, C2H3, C2H2, and C2H. Furthermore, CH2CHO, CH2CO, and HCCO are the intermediate particles for the oxidation of the hydrocarbons. CH2CHO can be produced by the reactions involving C2H4 and C2H2. HCCO is generated by the decomposition of CH2CO and the oxidation of C2H2. HCO and CO have complex generating pathways, as shown in Figure 13. Besides, both OH and HO2 can react with CO to

![Figure 10](https://dx.doi.org/10.1021/acsomega.0c04735)
produce CO$_2$, and CO + OH → H + CO$_2$ is the dominant reaction to consume CO.

Figure 14 shows the reaction pathways in the methane–air combustion with plasma assistance when the applied voltage amplitude is 11 kV. The red reaction is an important route existing only in the methane–air plasma-assisted combustion. This figure illustrates that though 84.7% of methane is consumed to form CH$_3$, 14.2% of methane reacts with CH by the reaction CH$_4$ + CH → C$_2$H$_4$ + H to generate C$_2$H$_4$, which is a new reaction path to form C$_2$H$_4$ in the plasma-assisted combustion. C$_2$H + H$_2$ → C$_2$H$_2$ + H can produce C$_2$H$_2$, which is an emerging pathway to form C$_2$H$_2$ in the plasma-assisted combustion. Except for the new reaction pathways occurring in the methane–air plasma-assisted combustion, the NPDBD plasma can change the contributions of the reaction paths. It can be seen that the contributions of the blue reactions in the combustion with plasma assistance are distinct from those without plasma assistance. The reactions involving active species such as the atom H play a significant role in the NPDBD plasma-assisted combustion, resulting in an obvious decrease in the densities of these active species, as shown in Figure 11.

3. CONCLUSIONS
The methane–air NPDBD plasma-assisted planar shear flow combustion is numerically investigated by combining the homemade plasma model with the combustion model based on software CHEMKIN-PRO. This work presents the following significant observations:

(1) The higher electric field enhances the processes of electron collision ionization, dissociation, and excitation, thereby producing more ions, radicals, and electronically excited species. As the applied voltage amplitude increases, the peak value of the discharge current density increases, and the peak of the discharge current density occurs earlier.

Figure 11. Mole fractions of (a) O, (b) H, and (c) OH in the methane–air planar shear flow combustions without and with plasma assistance under different amplitudes of the applied voltage.

Figure 12. Reaction pathway map of the methane–air NPDBD plasma when the applied voltage amplitude is 11 kV.
O is the active species of the highest particle density in the methane–air plasma.

The maximum temperature is around 2200 K when the applied voltage amplitude is 9 or 10 kV but decreases to around 1900 K when the applied voltage amplitude varies from 11 to 13 kV. The active species produced in the methane–air NPDBD plasma promote the chain-branching reactions by the kinetic effect, moving the flame upstream.

In the NPDBD plasma-assisted combustion, 14.2% of methane reacts with CH to generate C2H4, which is the new reaction pathway to form C2H4.

The NPDBD plasma can change the contributions of the reaction pathways in the methane–air combustion, in particular, the reactions involving active species such as H play a significant role in the plasma-assisted combustion, causing an obvious decrease in the densities of these active species with plasma assistance.

4. METHODS

The simulation model consists of the homemade one-dimensional plasma model and the two-dimensional combustion model based on software CHEMKIN-PRO. In previous studies, the plasma model has been implemented and validated for various NPDBD plasmas in different gas compositions.29–32 Figure 15 shows the schematic of the NPDBD plasma-assisted combustion system used in this work. The descriptions of the NPDBD plasma model and the planar shear flow combustion model are presented in Sections 4.1 and 4.2, respectively. The particle densities calculated by the plasma model are used as the initial particle densities of the combustion model. The combustion model is carried out on the basis of the CHEMKIN-PRO software platform combined with the reaction mechanism GRI-Mech 3.0.33 In the present model, the stoichiometric mixture methane–air is composed of 0.9CH4/2O2/7.52N2. The gas temperature is 400 K and the gas pressure is 760 mmHg. The overall gas flow rate is 20 cm/s.

4.1. NPDBD Plasma Model. The parameters of the NPDBD are set as follows. The applied voltage amplitude ranges from 9 to 13 kV. The pulsed voltage frequency is 10 kHz and the pulse width is 100 ns. The discharge gap distance and the dielectric layer thickness are 0.3 and 0.1 cm, respectively. The two dielectric layers are placed on the two
sides of the discharge gap. The relative permittivity of the dielectric is set to 4. The initial electron density is $10^7 \text{ cm}^{-3}$ and the neutral species density is $10^3 \text{ cm}^{-3}$. The secondary electron emission rate is 0.02. The boundary flux density of the electron at the dielectric material is determined by the secondary electron emission combined with the kinetic Maxwellian flux condition. The boundary flux densities of the ion and neutral species are only determined by the kinetic Maxwellian flux condition. The lower side of the dielectric layer is connected to the positive pole of the power supply, and the upper side of the dielectric layer is grounded.

The 87 species considered in the methane–air NPDBD plasma are listed in Table 1. The reaction equations and the corresponding rate coefficients are presented in the Supporting Information. The majority of electron collision reaction rate coefficients are calculated by BOLSIG+ using the cross-platform.

### Table 1. Species Considered in the Methane–Air NPDBD Plasma

| gas type | charged species | neutral species |
|----------|----------------|----------------|
| methane  | C$^+$, H$^+$, H$_2^+$, CH$^+$, CH$_2^+$, CH$_3^+$, CH$_4^+$, C$_2$H$^+$, C$_2$H$_2^+$, C$_2$H$_3^+$, C$_2$H$_4^+$, C$_2$H$_5^+$, e$^-$, H, CH$_2$ | C, H, H$_2$, CH, CH$_2$, CH$_3$, CH$_4$, C$_2$H, C$_2$H$_2$, C$_2$H$_3$, C$_2$H$_4$, C$_2$H$_5$, C$_3$H, C$_3$H$_2$, C$_3$H$_3$, C$_3$H$_4$, C$_3$H$_5$, C$_3$H$_6$, C$_3$H$_7$, C$_3$H$_8$, O, O$_2$, N, N$_2$, NO, NO$_2$, N$_2$O, N$_2$O$_2$, N$_2$O$_3$, N$_2$O$_4$, O(1D), O$_2$(A), N$_2$(B), N$_2$(C), OH, H$_2$O, H$_2$O$_2$, CO, CO$_2$, HNO, HNO$_2$, HNO$_3$, CHO, CH$_2$O, CH$_3$OH, CH$_3$OH, CN, HCN, C$_2$H$_5$ |
| air      | O$^+$, O$_2^+$, N$_2^+$, N$_2^+$, NO, NO$_2$, N$_2$O, N$_2$O$_2$, O(1D), O$_2$(A), N$_2$(B), N$_2$(C), e$^-$, O, O$_2$, O$_3$, O$_4$, O$_5$, O$_6$, O$_7$, NO, NO$_2$, NO$_3$, NO$_4$, NO$_5$, NO$_6$, NO$_7$, NO$_8$, NO$_9$, NO$_{10}$ | O, O$_2$, N, N$_2$, NO, NO$_2$, N$_2$O, N$_2$O$_2$, N$_2$O$_3$, N$_2$O$_4$, O(1D), O$_2$(A), N$_2$(B), N$_2$(C), OH, H$_2$O, H$_2$O$_2$, CO, CO$_2$, HNO, HNO$_2$, HNO$_3$, CHO, CH$_2$O, CH$_3$OH, CH$_3$OH, CN, HCN, C$_2$H$_5$ |
| methane/ | OH$^+$, H$_2$O$^+$, H$_2$O$^+$, e$^-$, OH$^-$ | OH, H$_2$O, H$_2$O$_2$, CO, CO$_2$, HNO, HNO$_2$, HNO$_3$, CHO, CH$_2$O, CH$_3$OH, CH$_3$OH, CN, HCN, C$_2$H$_5$ |
sections from the online database LXCat. The other reaction rate coefficients are taken from the literature.

The dynamic behaviors of the particles in the one-dimensional plasma model are determined by the continuity equation

$$\frac{\partial N_i}{\partial t} + \nabla \cdot \mathbf{\Gamma}_i = S_i$$  \hspace{1cm} (1)

where \( N \) is the particle density, subscript \( i \) denotes the \( i \)th species, \( \mathbf{\Gamma} \) is the particle flux density, and \( S \) is the particle source term. \( S \) is obtained by multiplying the reaction rate and the particle densities of the species present on the left-hand side of the reaction equation. Based on the drift–diffusion approximation, \( \mathbf{\Gamma}_i \) is described as the momentum equation

$$\mathbf{\Gamma}_i = Z_i \mu_i E \, N_i - D_i \nabla N_i$$  \hspace{1cm} (2)

where \( \mu \) is the mobility and \( D \) is the diffusion coefficient. For a neutral particle, only the diffusion term is considered in the momentum equation. Symbol \( Z \) equals 1 for positive ions and equals \(-1\) for electrons and negative ions.

The electric field intensity \( \mathbf{E} \) is calculated by the current conservation equation

$$\frac{\partial \mathbf{E}}{\partial t} = \frac{\mathbf{J}_0 - \mathbf{J}_e}{\varepsilon_0}$$  \hspace{1cm} (3)

where \( \varepsilon_0 \) is the permittivity of vacuum, \( \mathbf{J}_0 \) is the total current density, and \( \mathbf{J}_e \) is the conduction current density. \( \mathbf{J}_0 \) and \( \mathbf{J}_e \) are further expressed as

$$\mathbf{J}_0 = (\varepsilon_0 \frac{\partial V_a}{\partial t} + \int_0^t \mathbf{J}_e \, dx) \left( \frac{d_x}{\varepsilon_x} \right)$$

$$\mathbf{J}_e = q_e (Z \mathbf{\Gamma}_e - \mathbf{\Gamma}_e)$$

where \( V_a \) is the applied voltage, \( d_x \) is the discharge gap distance, \( d_x \) is the thickness of the dielectric layer, and \( \varepsilon_x \) is the relative permittivity of the dielectric.

The electron temperature \( T_e \) can be calculated by the following equations

$$\frac{\partial (\frac{3}{2} k_b T_e N_e)}{\partial t} + \nabla \cdot \mathbf{Q}_e = -q_e \mathbf{\Gamma}_e E - q_e \sum \Delta j_j r_j$$

$$\mathbf{Q}_e = -\frac{5}{2} k_b D_e N_e T_e + \frac{5}{2} k_b T_e \mathbf{\Gamma}_e$$

where \( k_b \) is the Boltzmann constant, \( \mathbf{Q}_e \) is the electron energy flux, \( \Delta j_j \) is the energy threshold of the \( j \)th electron–neutral inelastic reaction, and \( r_j \) is the reaction rate of the \( j \)th reaction.

The improved Scharfetter–Gummel algorithm is used to solve the above nonlinear equations. Kulikovsky has introduced detailed implement approaches of the improved Scharfetter–Gummel algorithm.\(^\text{46}\) The computer code is structured by FORTRAN.

4.2. Planar Shear Flow Combustion Model. The combustion model is carried out on the two-dimensional planar shear flow module of the CHEMKIN-PRO platform. A symmetric planar coordinate system is used to solve the module. The central line of the combustion tube is set as the zero point on the \( y \) axis in Figures 7–12. The temperature of the burner wall is set to 910 K. The length and the height of the shear flow burner are 200 and 1.2 cm, respectively.

Thermal and transport properties of various species as well as the combustion chemical reactions come from the mechanism GRI 3.0.\(^\text{33}\) The set of equations describing the combustion model are given as follows.

The momentum equation can be indicated as

$$\rho u \frac{\partial u}{\partial x} - \frac{\rho u}{m} (-\xi \rho V_{y_{\text{max}}}) \frac{\partial u}{\partial x} + \frac{\partial P}{\partial x} = \frac{\rho u}{m^2} \frac{\partial}{\partial x} \left( \rho c_{\text{p}} u^2 \frac{\partial u}{\partial x} \right)$$

where \( \rho \) is the mass density of a gas mixture, \( u \) is the axial velocity of a fluid mixture in the \( x \) direction, \( x \) is the spatial coordinate along the principal flow direction, \( m \) is the mass flux, \( \xi \) is the normalized stream function, \( \nu \) is the fluid velocity in the \( y \) direction, \( V_{y_{\text{max}}} \) is the maximum channel dimension, \( P \) is the gas pressure, and \( c_\text{p} \) is the mixture viscosity.

The state equation is expressed by

$$P = \frac{\rho R T}{W}$$  \hspace{1cm} (9)

where \( R \) is the universal gas constant and \( W \) is the mean molecular weight of the gas mixture.

The stream function \( \xi \) is expressed by

$$\xi = \frac{1}{m^2} \int_0^y \rho u \, dy$$  \hspace{1cm} (10)

where \( m' \) is the local mass flux and \( y \) is the cross-stream coordinate. The dynamics of the \( k \)th species in the combustion is determined by the species equation

$$\rho u \frac{\partial Y_k}{\partial x} - \frac{\rho u}{m} (-\xi \rho V_{y_{\text{max}}}) \frac{\partial Y_k}{\partial x} = \omega_k W - \frac{\rho u}{m} \frac{\partial}{\partial x} (\gamma y Y_k V_{k,y})$$

where \( Y_k \) is the mass fraction of the \( k \)th species, \( \omega_k \) is the chemical production rate of the \( k \)th species due to gas-phase reactions, and \( W_k \) is the molecular weight of the \( k \)th species.

The diffusion velocity \( V_{k,y} \) of the \( k \)th species in the \( y \) direction is given by

$$V_{k,y} = -\frac{D_{\text{im}} \rho u y}{X_k m} \frac{\partial X_k}{\partial y} - \frac{D_{t} \rho u y}{X_k m} \frac{\partial T}{\partial y}$$

where \( D_{\text{im}} \) is the mixture-averaged diffusion coefficient of the \( k \)th species, \( X_k \) is the mole fraction of the \( k \)th species, and \( D_{t} \) is the thermal diffusion coefficient of the \( k \)th species.

The energy equation is described as

$$\rho c_{\text{p}} \frac{\partial T}{\partial x} - \frac{\rho c_{\text{p}}}{m} (-\xi \rho V_{y_{\text{max}}}) \frac{\partial T}{\partial x}$$

$$= \frac{\rho u}{m^2} \frac{\partial}{\partial x} \left( \rho c_{\text{p}} u^2 \frac{\partial T}{\partial x} \right) - \sum \omega_k W_k h_k$$

$$- \frac{\rho c_{\text{p}}}{m} \sum Y_k V_{k,y} c_{\text{p}k} \frac{\partial T}{\partial y}$$

where \( T \) is the temperature, \( c_{\text{p}} \) is the specific heat of the gas mixture at constant pressure, \( c_{\text{p}k} \) is the specific heat capacity of the \( k \)th species at constant pressure, \( h_k \) is the specific enthalpy of the \( k \)th species, and \( \lambda \) is the thermal conductivity of the gas mixture.
Postdoctoral Science Foundation (No. 2017M612324). This work was supported by the National Natural Science Foundation of China (No. 51707111) and the China Postdoctoral Science Foundation (No. 2017M612324).

ACKNOWLEDGMENTS

The authors declare no competing financial interest.

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