

2-D numerical modeling of flame behavior under electric field effect

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ABSTRACT

In this work, premixed turbulent combustion of methane under the effect of the electric field was simulated using Ansys /Fluent with Gri-mech 1.2. The simulation included Ionic species and NO formation.

The combustion simulation without electric field was done first to validate the mathematical model for laminar combustion. It was found that flame conic shape and adiabatic flame temperature agree with the results of previously published work.

The combustion simulation of the flame under electric field effect, includes modeling of the electric field equation, which was implemented in Fluent using user-defined sources (UDS) coupled with user-defined functions (UDFs).

It was found that H_3O^+ and CHO^+ species are consumed immediately after their production as a result of electric field effect. On the other hand, the flame stability was enhanced. Emitted pollutants were minimized with a little reduction in CO concentration, which agrees with previously published experimental work.

1. INTRODUCTION

Improving combustion process to minimize the emitted pollutants is a major trend in the field of combustion research. One of those improvements that may reduce the pollutants formation is to control the flame behavior using an electric field, which may also stabilize the flame. The interaction phenomena between the flame and electric field was addressed earlier [1], but is still not fully understood. Recent studies have been conducted to discuss such effect on combustion characteristics [2-3]. The stabilization of premixed laminar Bunsen flames under the effect of AC electric field with low frequency was studied by Kim, et al. [4]. Yanlai Luo et al. [5] investigated the effect of DC electric field on a small ethanol diffusion flame. They found that the applied electric field changes the flame characteristics mainly due to the body forces acting on charged particles in the electric field. In the same context Yunhua Gan et al. [6] studied experimentally the effect of Alternating Current (AC) electric field on flame behaviors of ethanol in small-scale.

The bi-ionic wind effect (ionic wind effects from positive and negative ions) explained the behavior of blow-off velocity with AC frequency in the low-frequency region. In their study on the effect of ionic wind on structure and temperature of laminar premixed flames influenced by electric fields, Johannes Kuhl et al. [7] found that the electric field leads to increased fresh gas and maximum flame temperatures and that this effect is most distinct for rich premixed flames.

The effect of electric field on the stability of lean methane-oxygen air was investigated by Tomcik, et al. [8], while the lift-off of propane flame under the effect of the electric field was discussed by Hutchins, et al. [9]. The polarity and electrode location effects on lift-off were also discussed in

their work.

Chemi-ionization and other ionization mechanisms in hydrocarbon and non-hydrocarbon flames were investigated by Fialkov [10]. The ions in methane, benzene, acetylene, saturated hydrocarbons C3-C8, alcohols, Ketone, ether, acetic acid, and CO flames were also investigated. The methodology and apparatus used for investigation of charged species in flames were also discussed. Calcote, [11] discussed and reviewed ions formation in flames whereas ions in flames were investigated by several researchers [12-15]. The electron concentrations of hydrocarbons, esters, alcohols, ethers and ketones flames at reduced pressure were studied by Bulewicz and Padley [16]. The kinetic processes in plasma (Ions, electrons, charged and neutral carbon clusters and nanometer particles) formed in hydrocarbon flames were examined by Starik, et al. [17].

In hydrocarbon flames, the main mechanism for ions formation is chemi-ionization. In this process, the large energy of the reaction ionizes a natural element in the products. This process happens in the elementary reactions in the detailed chemical mechanism. H_3O^+ ion and smaller concentrations of CHO^+ were found in hydrocarbon flames [12].

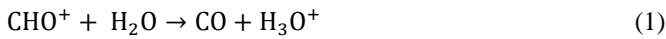
It is seen from above that no complete theoretical investigation with valid 2-D numerical model was done for both laminar and turbulent combustion with electric field effect. Furthermore, most previous work was experimental. The objective of this work is to study premixed flames behavior and their stability under the effect of an electric field. To do so, premixed combustion simulations with and without electric field effect were carried out using Ansys/Fluent software. The new implementation in this work is the coupling of premixed turbulent combustion simulation by Ansys/Fluent with the electric field equation. Up to the best of the author's

knowledge, flame behavior under electric field effect was not simulated before, with the coupling of premixed combustion simulation by Ansys/Fluent with the electric field equation.

2. PHYSICAL MODEL

2.1 Ionic species

The presence of an electric field alters the behavior of flames due to the existence of ionic species in their detailed chemistry. So, the electric field effect on pollutant emissions, flame stability, flame speed, flame luminosity and flame shape were discussed in the literature in order to improve combustion process. In addition, a feedback control procedure for flame control with the electric field as an actuator was suggested to highlight the importance of control engineering in this field. There are many mechanisms that are responsible for ions formation in flames such as electron transfer, ionization by collision, chemi-ionization and excitation energy transfer. In hydrocarbon-air flames, H_3O^+ ion is produced by the reaction [18]:



While CHO^+ ion is produced by the following reaction [18]:



But, H_3O^+ is consumed by another reaction:



2.2 Ionic wind in flames

The electric charges placed into an electric field are affected by the field with an electric force called Coulomb force. An electric field applied to flame make electrons move from reaction region to the positive electrode. Similarly, the positive ions move but in the opposite direction. Some of the positive ions collide with the natural species, resulting in the transfer of ions momentum to species. This creates a hydrodynamic pressure on the flame which is called the ionic wind. This process is demonstrated in Fig. 1.

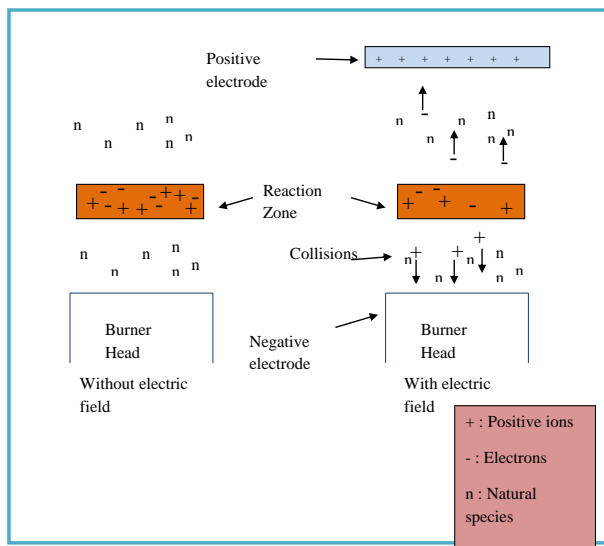


Figure 1. A demonstration of the ionic wind effect

Another important process happens, along with the ionization, is the recombination process. This process eliminates the produced ions in the reaction zone. Without an electric field, a state of balance (equilibrium) between recombination and ionization processes took place. By applying an electric field, some of the ionic species will be extracted from the reaction zone and a current of ions will be created. The interaction between electric fields and flames was discussed in [19].

3. MATHEMATICAL MODEL

The combustion simulation without electric field was done first to validate our mathematical model. The conducted simulation includes two methods for modeling: premixed turbulent combustion by Fluent, and premixed laminar combustion simulation by Fluent with Gri mech 1.2. It was found that flame conic shape and adiabatic flame temperature agree with the results of previously published work of laminar combustion [21-24].

The combustion of premixed turbulent flame under electric field effect, including the ionic species and NO formation, was simulated by Fluent with Gri mech 1.2. The electric field equation was implemented in Fluent by UDS and coupled with the simulation by UDFs which were written in C-Language. These UDF are presented in Table 3 and Table 4.

3.1 Governing Equations

Modeling premixed laminar and turbulent combustion is done by solving the governing equations of continuity, momentum, energy and species equations along with turbulent flow equations from the appropriate turbulent model such as k-ε. In addition, a turbulent chemistry model is required to include the effects of turbulence on the production rate of species in the main species equations such as eddy dissipation concept (EDC) model [20]. The transient terms ($\frac{\partial y}{\partial t}$) for all the equations must be dropped in these models since the simulations were based on steady state cases. The continuity equation (mass conservation) for 2D axisymmetric is [25, 26]: The mass source (S_m) in this model is zero.

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho v_x)}{\partial x} + \frac{\partial(\rho v_r)}{\partial r} + \frac{\rho v_r}{r} = S_m \quad (4)$$

The momentum equations for 2D axisymmetric are [25, 26]:

$$\frac{\partial(\rho v_x)}{\partial t} + \frac{1}{r} \frac{\partial(r \rho v_x v_x)}{\partial x} + \frac{1}{r} \frac{\partial(r \rho v_x v_r)}{\partial r} = - \frac{\partial p}{\partial x} + \frac{1}{r} \frac{\partial}{\partial x} \left[r \mu \left(2 \frac{\partial v_x}{\partial x} - \frac{2}{3} (\nabla \cdot \vec{v}) \right) \right] + \frac{1}{r} \frac{\partial}{\partial r} \left[r \mu \left(\frac{\partial v_x}{\partial r} + \frac{\partial v_r}{\partial x} \right) \right] + F_x \quad (5)$$

$$\frac{\partial(\rho v_r)}{\partial t} + \frac{1}{r} \frac{\partial(r \rho v_x v_r)}{\partial x} + \frac{1}{r} \frac{\partial(r \rho v_r v_r)}{\partial r} = - \frac{\partial p}{\partial r} + \frac{1}{r} \frac{\partial}{\partial r} \left[r \mu \left(2 \frac{\partial v_r}{\partial r} - \frac{2}{3} (\nabla \cdot \vec{v}) \right) \right] + \frac{1}{r} \frac{\partial}{\partial x} \left[r \mu \left(\frac{\partial v_x}{\partial r} + \frac{\partial v_r}{\partial x} \right) \right] - 2 \mu \frac{v_r}{r^2} + \frac{2}{3} \frac{\mu}{r} (\nabla \cdot \vec{v}) + \rho \frac{v_z^2}{r} + F_r \quad (6)$$

The external body forces (F_x and F_r) are zero, and the swirl velocity (v_z) is also zero. While the term $\nabla \cdot \vec{v}$ is given by [25, 26]:

$$\nabla \cdot \vec{v} = \frac{\partial v_r}{\partial r} + \frac{\partial v_x}{\partial x} + \frac{v_r}{r} \quad (7)$$

The energy equation is [25-26]:

$$\frac{\partial(\rho E)}{\partial t} + \nabla \cdot (\vec{v} (\rho E + p)) = \nabla \cdot (k_{eff} \nabla T - \sum_j h_j \vec{J}_j + (\bar{\tau}_{eff} \cdot \vec{v})) + S_h \quad (8)$$

The effective thermal conductivity (k_{eff}) is the sum of turbulent thermal conductivity and the normal one ($k + k_t$). The third term in the equation ($\bar{\tau}_{eff} \cdot \vec{v}$) represents the viscous dissipation. \vec{J}_j represents the diffusion flux of species j . The S_h term includes the heat of chemical reactions. For a complete set of equations regarding enthalpy, diffusion, ions, species, NO formation, mixture density, thermal conductivity, viscosity and $k-\epsilon$ model of turbulence, please refer to Ansys/Fluent user's guide [26].

3.2 Modeling electric field and the coupling terms

The electric field equation is given by Gauss's law of electrostatic which is:

$$\nabla^2 V = -\rho_v \quad (9)$$

where the volumetric charge is given by:

$$\rho_v = e \frac{(n^+ - n^-)}{\epsilon_0} \quad (10)$$

where ϵ_0 is the vacuum permittivity. The electric field is related to voltage by:

$$\mathbf{E} = -\nabla V \quad (11)$$

The coupling term for the momentum equation is given by (a volumetric source to the equation):

$$F_i = e E_i (n^+ - n^-) \quad (12)$$

The heat from the electric field is a model as a volumetric source to the energy equation which is given by:

$$S_h = \sum_{k=1}^{N_c} e n^k S^k E_j (v_j + V_j^k) \quad (13)$$

where N_c is the number of ions and n^k is the concentration of ion k [21]. For the ionic species equations, the coupling term (for each ion) is added to the diffusion flux equation so it becomes:

$$\vec{J}_i = -\rho D_{i,m} \nabla Y_i - D_{T,i} \frac{\nabla T}{T} - \rho Y_i z_i u_{m,i} F \nabla V \quad (14)$$

where z_i is the charge number and $u_{m,i}$ is the mobility of species.

4. COMBUSTION WITHOUT ELECTRIC FIELD

4.1 Laminar combustion

The modeling procedure included the coupled solver in this model to solve momentum and continuity equations simultaneously. For boundary conditions, the inlet temperature is 298 K and the equivalence ratio is one (air and methane). The inlet velocity is 25 m/s and the turbulent intensity is 5%. The walls are adiabatic (zero heat flux). The pressure at the outlet is zero (gauge pressure).

The CH_4 mass fraction contour is shown in Figure 2. The flame shape is a cone which is the predicted shape. The adiabatic temperature contour is shown in Figure 3. The maximum temperature reached 1740 K, which is in the normal range for methane combustion.



Figure 2. The CH_4 mass fraction



Figure 3. The adiabatic flame temperature contour

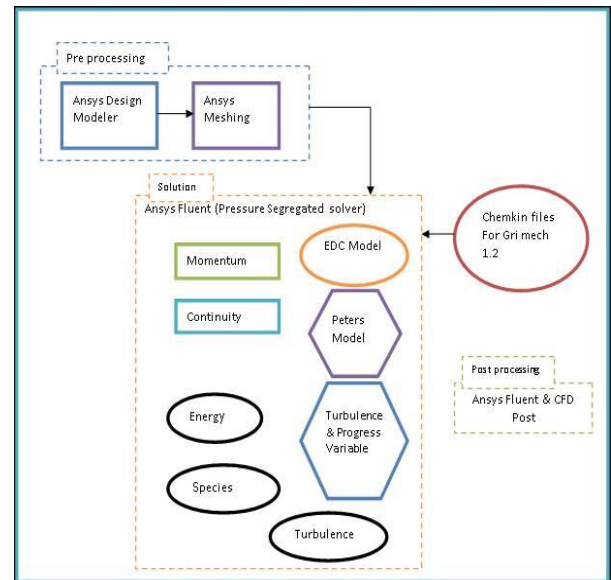


Figure 4. The modeling procedure for premixed turbulent combustion

4.2 Turbulent combustion

The simulations procedures for the two approaches (EDC and Peters) are shown in Figure 4. The Ansys Fluent and Ansys CFD post were used for post-processing. The geometry is a single hole burner (2D- axisymmetric) and it is shown in Figure 5. The value of H1 is equal to 350 mm, where V_1 and V_2 are equal to 10 and 30 mm respectively. The mesh of the geometry is shown in Figure 6. The number of nodes is 3267 and the number of elements is 3120. The geometry was made

by Ansys Design Modeler, while Ansys meshing tool was used to mesh the geometry. A grid independent test was performed to ensure that the mesh sizes are considered to produce identical results. The mesh size is refined at the fuel and air inlet to produce the most accurate numerical results. For the chemical mechanism, the GRI-mech 1.2 Chemkin file was imported to Fluent. The temperature contour is shown in Figure 7. The mass fraction contour for CH₄ is shown in Figure 8. The maximum adiabatic temperature was 2310 K which is in the adiabatic temperature range of methane combustion. The adiabatic temperature in this model also agrees with [22-24]. The maximum temperature was 2222 K at an inlet temperature of 298 K and 1 bar pressure for stoichiometric combustion.

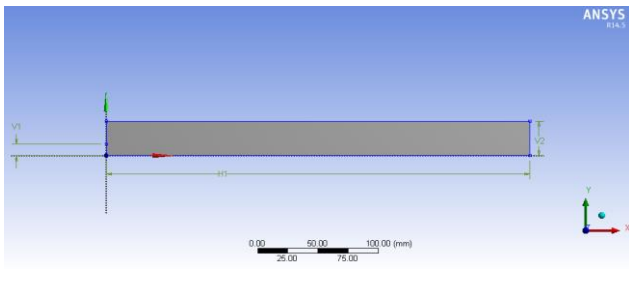


Figure 5. The burner geometry

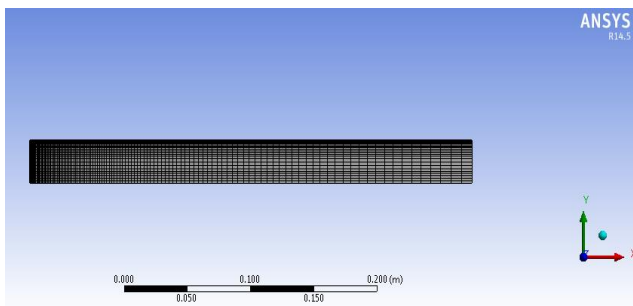


Figure 6. The mesh for the burner

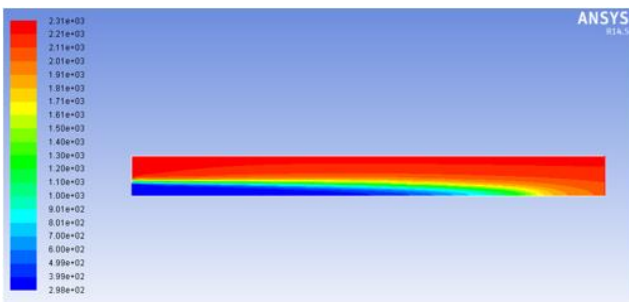


Figure 7. The temperature contours

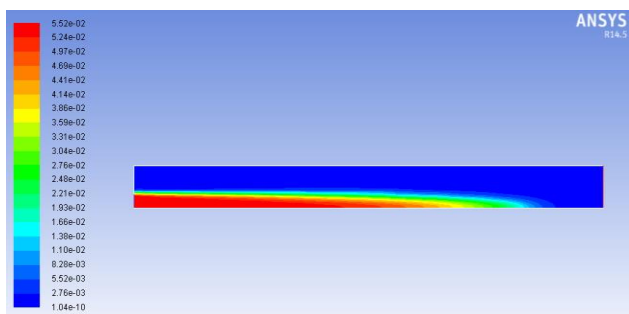


Figure 8. CH₄ mass fraction contours

5. COMBUSTION RESULTS UNDER ELECTRIC FIELD EFFECT

This section presents a simulation of premixed turbulent combustion with Grimech 1.2 mechanism under electric field effect, presented by UDS in Fluent. Fluent can be coupled with electromagnetic fields model by many methods. The method implemented here considered UDF (User Defined Function) module in Ansys/Fluent to define the momentum and heat sources. The mesh and geometry are the same as before. The UDS in Fluent was used to define the PDE for the electric field. The outlet of the burner was assumed to be the positive electrode while the wall near the inlet was assumed to be the negative electrode.

The electrical voltage by Fluent is shown in Figure 9.

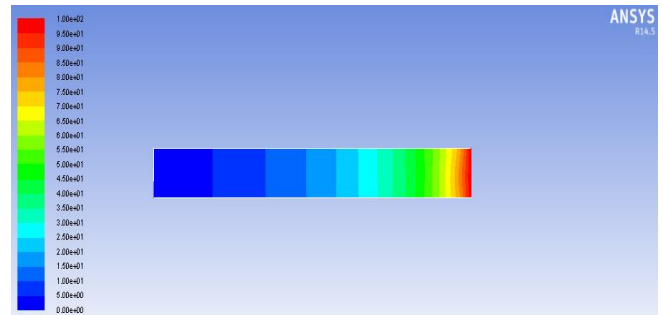


Figure 9. The voltage contours by Fluent

The positive electrode voltage was 1 kV. The UDF in Fluent is used to define three sources for momentum and electric field equations. The first source was added to the first momentum equation (The Momentum in the axial direction). The second source was added the to the second momentum equation (In the radial direction). The difference in code between the two sources returns the radial component of the gradient of the voltage. The third source was added to the electric field equation.

Table 1. Maximum values of combustion species under electric field effect

Variable name	Maximum values
Pressure (gauge)	9.20373 Pascal
Velocity Magnitude	20.3237 m/s
Molar concentration of CO	9.344763×10^{-5} kmol/m ³
Mole fraction of NO	7.13308×10^{-4}
Molar concentration of OH	4.302085×10^{-5} kmol/m ³
Molar concentration of O	2.119532×10^{-5} kmol/m ³
Molar concentration of CO ₂	4.730764×10^{-4} kmol/m ³

Table 2. Maximum values of combustion species (without electric field effect)

Variable name	Maximum values
Pressure (gauge)	9.190816 Pascal
Velocity Magnitude	20.32314 m/s
Molar concentration of CO	9.404726×10^{-5} kmol/m ³
Mole fraction of NO	7.117746×10^{-4}
Molar concentration of OH	2.121053×10^{-5} kmol/m ³
Molar concentration of O	4.308933×10^{-5} kmol/m ³
Molar concentration of CO ₂	4.731025×10^{-4} kmol/m ³

Table 3. The code for the first source with description

Code	Description
#include "udf.h"	Import the UDF library
DEFINE_SOURCE(First_momentum_source, cel, th, dS, eqn) {	Define the function (source)
const real E_charge = 1.60217657e-19;	Declare and define constant (Electron charge)
const real Avog_number = 6.022e23;	Declare and define constant (Avogadro number)
const real MW_H3O = 19.0232;	Declare and define constant (H_3O^+ molar mass)
const real MW_CHO = 29.0180;	Declare and define constant (CHO^+ molar mass)
Real Density_number_H3O, Density_number_CHO, source;	Declare variables (Density numbers and source variables)
Density_number_H3O= 1000*Avog_number*C_YI(cel,th,33)*C_R(cel,th)/MW_H3O;	Define density number of H_3O^+ by: $n_i = \frac{(1000)(Avg. num.)Y_i\rho}{MW_i}$
Density_number_CHO= 1000*Avog_number*C_YI(cel,th,32)*C_R(cel,th)/MW_CHO;	Define density number of CHO^+ by: $n_i = \frac{(1000)(Avg. num.)Y_i\rho}{MW_i}$
source= -1*C_UDSI_G(cel,th,0)[0]*E_charge*(Density_number_H3O + Density_number_CHO);	Define the source by: $Source = -E_{axial}e(n_{H_3O^+} + n_{CHO^+})$
return source;	Return the source

Table 4. The code for the third source with description

Code	Description
#include "udf.h"	Import the UDF library
DEFINE_SOURCE(ElectricField_source, cel, th, dS, eqn) {	Define the function (source)
const real E_charge = 1.60217657e-19;	Declare and define constant (Electron charge)
const real Avog_number = 6.022e23;	Declare and define constant (Avogadro number)
const real MW_H3O = 19.0232;	Declare and define constant (H_3O^+ molar mass)
const real MW_CHO = 29.0180;	Declare and define constant (CHO^+ molar mass)
Real Density_number_H3O, Density_number_CHO, source;	Declare variables (Density numbers and source variables)
Density_number_H3O= 1000*Avog_number*C_YI(cel,th,33)*C_R(cel,th)/MW_H3O;	Define density number of H_3O^+ by: $n_i = \frac{(1000)(Avg. num.)Y_i\rho}{MW_i}$
Density_number_CHO= 1000*Avog_number*C_YI(cel,th,32)*C_R(cel,th)/MW_CHO;	Define density number of CHO^+ by: $n_i = \frac{(1000)(Avg. num.)Y_i\rho}{MW_i}$
source = E_charge*(Density_number_H3O + Density_number_CHO)	Define the source by: $Source = e(n_{H_3O^+} + n_{CHO^+})$
return source;	Return the source

The velocity magnitude does not differ largely from the magnitude under the effect of electric field. The deceleration due to applying the electric field was negligible.

It was noticed that while the concentration of NO increases with an electric field, the total overall concentration of NO_x (NO+NO₂) decreases under electric field effect [23]. The same behavior was obtained and presented in tables 1 and 2, NO concentration was increased by applying the electric field. The rise of temperature in this region tends to increase the rate of formation of NO, since the latter is very sensitive to the flame temperature. A few tens of ppm of hydrocarbon in the presence of sufficient oxygen can quantitatively convert NO to NO₂. The flame stability was enhanced. The enhanced stability minimized the emitted pollutants. A little reduction in CO concentration was achieved, which agree with the results of previously published experimental work [21-24]. CO concerning reduction using electric field is based on the assumption that unburned hydrocarbons are also reduced due to the application of an electric field as a result of reducing the gap between the flame and the burner rim. By reducing the gap between the reaction zone and burner rim the electric field converts a certain part of that region where incomplete combustion occurs into a region of complete combustion.

6. CONCLUSIONS

To achieve the main objective of this study, simulation of premixed turbulent combustion was conducted. The method implemented in this research considered UDF (User Defined Function) module in Ansys/Fluent to define the momentum and heat sources. The used mesh has 3267 nodes and 3120 elements. The UDS in Fluent was used to define the PDE for the electric field. The maximum adiabatic temperature was 2310 K which agrees with literature. The simulation included the ionic species and NO formation with electric field effect. NO concentration was increased by applying the electric field due to the increase in the flame temperature. It was found that H_3O^+ and CHO^+ species were consumed immediately after their production as a result of electric field effect. On the other hand, the flame stability was enhanced as a result of reducing the gap between the flame and the burner rim. Consequently, emitted pollutants were minimized and a little reduction in CO concentration was achieved.

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