

Numerical simulation of ethylene combustion characteristics under a new double-layer porous media burner

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Abstract: The efficient use of energy is an important strategic issue concerning our energy security and double carbon goals. Many industrial waste gases, such as oil refineries, contain a lot of ethylene, which is a gas that is harmful to people and the environment. The use of high-efficiency burners to reduce ethylene emissions is a proven and convenient way, so the improvement and optimization of high-efficiency burners has become a hot research issue nowadays. In this paper, a new porous media burner is designed, and a numerical model of the structure is established based on finite element software. The porous media burner is used to treat low calorific value ethylene and effectively reduce the direct emission of low calorific value ethylene in wastewater treatment and chemical industries. Based on the model, the combustion characteristics and pollutant emission characteristics of premixed gas at different equivalence ratios and different flow rates were investigated. The results show that the maximum combustion temperature can reach 1757K with a constant inlet flow rate of premixed gas and a full combustion at an equivalent ratio of 0.85; the maximum temperature increases rapidly with the increase of flow rate at an inlet flow rate of 0.65-0.85 m/s with a constant equivalent ratio, and the temperature rise effect increases slowly when the flow rate is higher than 0.85 m/s; the new porous media The maximum reduction of pollutant emissions of the new porous media burner reaches 37.9%. This study has a guiding effect on the design and engineering application of porous media combustion devices.

1. Introduction

In recent years, China's GDP has been growing at a high rate of nearly 7% per year. Coupled with human's attention to the environment and global warming, our demand for clean energy is also increasing. Porous medium combustion technology is a relatively novel combustion technology, compared with the traditional boiler combustion, pulsating combustion, catalytic combustion, high temperature air combustion. Because of its good combustion stability, can significantly expand fuel lean combustion limit, can reduce pollutant emissions, high combustion efficiency and many advantages, it is widely used in heat exchange materials, automobile exhaust treatment, industrial waste gas treatment and heat recovery and other fields.

Porous medium materials have unique combustion characteristics. The high temperature flue gas generated by flame combustion will heat the porous medium solid and form a preheating zone in the upstream of the combustion zone. The preheating zone preheats the newly added ethylene premixed gas through gas-solid heat

conduction, radiation heat transfer and convection heat transfer, so that the gas quickly reaches the required combustion temperature and promotes the subsequent combustion zone to burn more fully, To exothermic stability, inhibit the production of toxic and harmful gases.

The combustion of premixed gas in porous media was first proposed by Weinberg P. With the help of the reflux characteristics of the burner, the heat released from the reaction can preheat the unreacted gas by means of heat conduction and heat transfer, which greatly improves the combustion efficiency. Subsequently, the combustion characteristics of porous media have been studied by many researchers at home and abroad. Jugjai and Rungsimuntuchart [6] applied the concept of combustion in porous media to improve the efficiency of thermal recirculation domestic gas burners. They constructed a new semi-enclosed porous radiant cycle burner, which improved the thermal efficiency of the new gas stove by about 12% compared with the traditional thermal efficiency. Barra et al. used a one-dimensional two-temperature unsteady model to focus on the influence of porous material properties on flame stability. Hsu et al. conducted a series of experimental and numerical

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simulation studies on combustion in a double-porous medium burner. Considering the influence of gas-solid phase heat transfer and solid radiation in the double-porous medium, Peters simplified reaction mechanism and one-dimensional steady state calculation method were used to study the flame propagation velocity and its influencing factors in the double-porous medium. Wang Di [10] studied the flame stability mechanism and radiation characteristics of porous media surface combustion flame based on flame stability mechanism and radiation characteristics. Zhu Rongjun et al. [11] found through numerical simulation that the flame temperature distribution of metal fiber surface combustion mode containing porous medium was more uniform and the local reaction heat release rate was lower. Shi Junrui et al. [12] invented a cylindrical radiant porous medium heater with diffusion combustion in the cavity. By taking advantage of the good radiative heat transfer performance of the porous medium, the heat transfer is more uniform, and the fuel with low concentration and low calorific value can be burned, which is more widely used.

Through the above analysis, it can be found that the current research on the multi-space medium burner is more focused on the combustion mechanism and characteristics, and there is a lack of research on the burner structure improvement to improve combustion efficiency and reduce toxic and harmful gases. In this paper, a new porous medium burner model is designed based on the

characteristics of the porous medium with good heat storage, radiation conduction and backflow preheating in the combustion zone. Using ethylene as fuel, the existing burner structure is improved to explore the advantages of the improved porous medium burner in terms of caloric value and pollutant emission. The advantages of this burner model and traditional burner in calorific value and fuel saving are verified by comparison.

2. Numerical Model

2.1 Physical model

The combustion of porous media is mainly single-layer combustion, double-layer combustion and reciprocating combustion. At present, the structure of double-layer porous media burner widely used in domestic and foreign studies is shown in Figure 1. It is filled by homogeneous porous media evenly, and the left and right sections are connected by porous media with different porosity. The small hole medium area is the preheating zone of combustion, and the filler material is alumina. The large porous medium area is used as the combustion zone. The main material is silicon carbide, and the physical parameters are shown in Table 1. The physical model of a new porous medium burner designed in this study is shown in Figure 2.

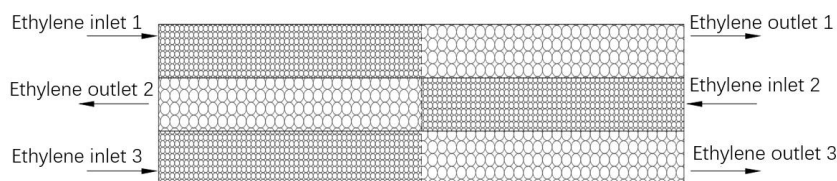


Figure 1 Double porous media burner before improvement

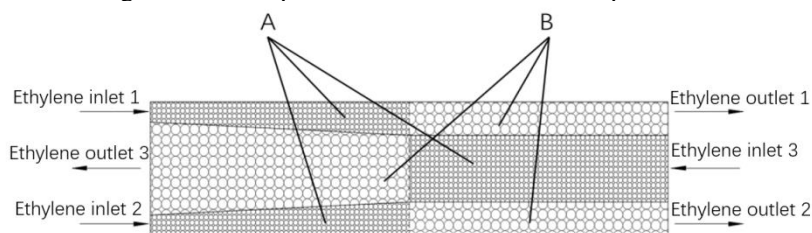


Figure 2 Double porous media burner improved

The improved burner is composed of two layers inside and outside, in which area A is the preheating zone, the filling material is set as small hole medium for the convenience of heat transfer, area B is the combustion zone, this area is set as large hole medium for speeding up the combustion. The premixed gas at gas inlet 1 and 2 is preheated by the high temperature combustion gas near gas outlet 3, thus improving the combustion efficiency of premixed gas during combustion. Among them, the

inclined transition of gas inlet 1 and 2 is set to further extend the length of the heating zone and increase the temperature of premixed gas in the preheating zone. The gas temperature at the inlet is the lowest, and a smaller pipe diameter can make this part of gas warm up quickly and preheat. The gas outlet 3 is the combustion zone, and the pipe diameter gradually expands, which can further promote the full combustion of premixed gas.

Table 1 Structure and physical parameters of a new porous media burner

	Orifice part	Macroporous part
determination of porosity	0.835	0.87

bore diameter (PPC)	25.6	3.9
Thermal conductivity(W/(m· K))	0.2	0.1
zone length	0.12	0.1

2.2 Mathematical model

The combustion of porous media can produce violent chemical reactions, causing tight coupling processes between gas-gas and gas-solid, It involves heat conduction, radiation and convection and other different heat exchange processes, so the simulation of the real condition is very complicated. This paper focuses on the preheating and combustion process from the point of view of analyzing the key factors and ignoring the secondary factors, and compares the burner model designed in this paper with the traditional burner. Boundary conditions and initial conditions need to be simplified and assumed as follows:

- (1) The porous medium does not catalyze the combustion process;
- (2) premixed gas has been fully mixed before entering the preheating zone;
- (3) The porous medium is set to be isotropic with uniform dispersion structure;
- (4) The reactants and products before and after combustion are incompressible ideal gases;
- (5) The whole burner ignores the influence of gravity.

Based on the above assumptions, the continuity equation in the numerical simulation is:

$$\frac{\partial(\rho\varepsilon)}{\partial t} + \frac{\partial(\rho\varepsilon\mu_i)}{\partial x_i} = 0 \quad (1)$$

Among them, the ρ after mixing the density of the gas; ε for the porosity of porous media; μ_i for velocity vector. The momentum conservation equation is :

$$\begin{aligned} & \frac{\partial(\rho\varepsilon\mu_j)}{\partial t} + \frac{\partial(\rho\varepsilon\mu_i\mu_j)}{\partial x_i} \\ & - \frac{\partial}{\partial x_i} \left(\rho\varepsilon V \frac{\partial\mu_j}{\partial x_i} \right) \\ & = - \frac{\partial(\varepsilon P)}{\partial x_j} - \frac{\mu\varepsilon^2}{K_p} \mu_j \\ & + \frac{\partial}{\partial x_i} \left[\rho\varepsilon V \left(\frac{\partial\mu_i}{\partial x_j} \right. \right. \\ & \left. \left. - \frac{2}{3} \frac{\partial\mu_k}{\partial x_k} \delta_{ij} \right) \right] \end{aligned} \quad (2)$$

Type, K_p for the permeability of porous medium; V as viscous resistance coefficient; μ for inertial resistance coefficient. The heat transfer between porous media is expressed by solid-phase energy equation:

$$\partial[(1-\varepsilon)P_s C_s T_s] / \partial t = \Delta(\gamma_e e^s \Delta T_s) + h\nu(T_g - T_s) \quad (3)$$

Among them, the γ_e^s as effective heat transfer coefficient of the porous medium material, $\gamma_e^s = \gamma_e^c + \gamma_e^r \gamma_e^c$, γ_e^c for reduction of heat transfer coefficient of radiation. P_s for porous medium density, C_s said the heat capacity of the materials, T_s for porous medium temperature.

In the combustion process, each component gas is regarded as an incompressible ideal gas, then the ideal gas equation of state is:

$$\rho_V = nRT \quad (4)$$

Type, n as the average molecular weight of the mix; R is the gas constant.

2.3 Calculation method and grid independence verification

In this paper, based on fluid simulation software FLUENT, the governing equations were discretized and solved, and the gas-solid energy equations were opened to ensure that the high temperature in the flame zone of the porous medium burner could be transferred to the solid medium.

In order to ensure good convergence of calculation results, sub-lack iteration is adopted, and the residual of energy equation is set as 1.0E-6, and the residual of other variables in this experiment is set as 1.0E-3[13]. The control volume method is used to discretize each conservation equation, and the SIMPLE algorithm is used to solve the momentum equation based on the pressure-velocity coupling.

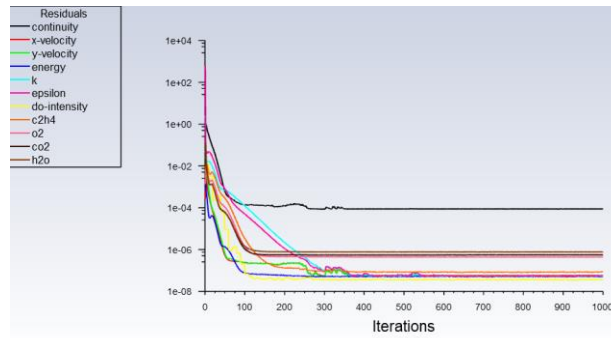


Figure 3 Calculating and solving the iterative process

Discretization error is one of the main sources of error between numerical calculation and experiment. In calculation, the discrete error will decrease with the thinning of the grid, but the thinning of the grid will lead to the increase of discrete points, resulting in a larger rounding error. Therefore, the number of grids is not the more the better. The optimal number of grids should be selected according to the numerical calculation results of multiple groups to ensure that the size of grid cells has little influence on the numerical calculation results, namely, grid independence analysis.

In this paper, the maximum temperature of the inner tube of the burner is selected as the solution objective. When the temperature does not change significantly with the change of the mesh cell size, it can be considered that the accuracy of the solution results is independent of the mesh cell size. C₂H₄/air equivalent ratio of 0.55 and inlet flow rate of 0.85m/s were selected as the working conditions for testing grid independence. After calculating the relationship between the size of grid cells, the number of grid nodes and the model temperature, see Figure.4.

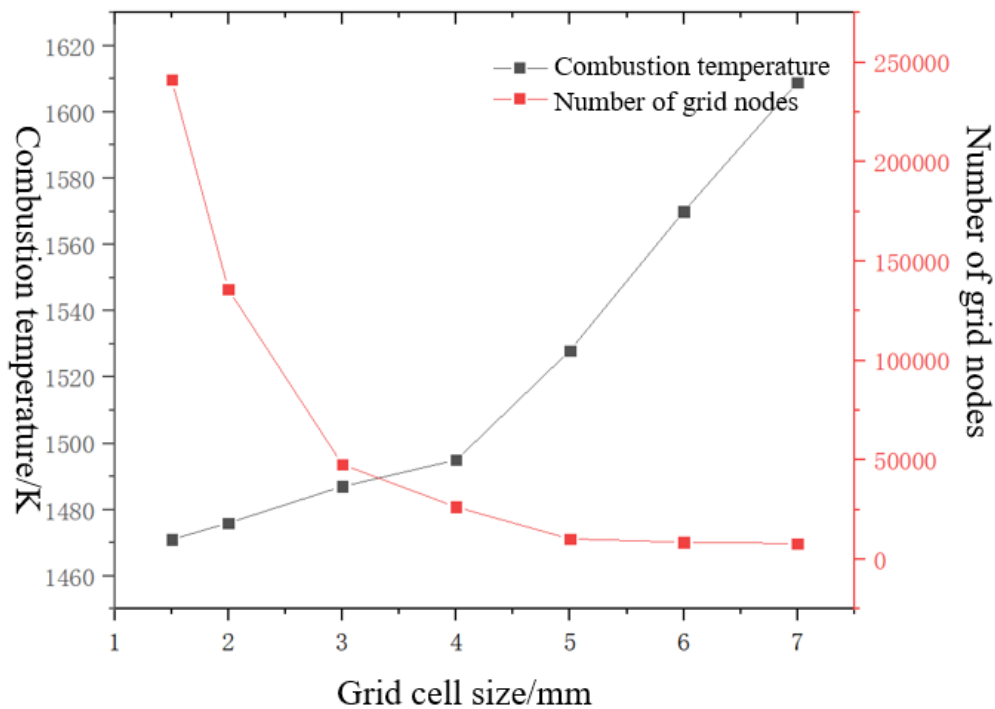


Figure 4 The grid independence

As can be seen from Figure 4, the number of grid nodes increases sharply with the refinement of the mesh cell size. When the mesh cell size is less than 3mm, the combustion temperature tends to be stable, and the calculation results at 2mm are basically the same as those at 1.5mm. Therefore, the maximum cell size was set to 2mm, and a total of 134,364 grids were generated after partitioning.

As the temperature of the whole combustion region changes dramatically during the combustion reaction process, the heat capacity of alumina pellets in the small-hole medium preheating zone is 1298J/(kg×K) in the literature [14] and the functional relationship between the effective thermal conductivity of alumina and temperature provided in the literature [15]:

$$k_s = 0.34691 - 736.72 \times 10^{-6}T + 1.2052 \times 10^{-6}T^2 \quad (5)$$

2.4 Selection of thermal property parameters

2.5 Setting of boundary conditions

Set the initial temperature and C2H4/air premixed gas velocity at the burner inlet. In order to ensure the stability of the calculation results and accelerate the convergence, the initial temperature was set to 1600K. This temperature

is relatively high, equivalent to setting up a high temperature device for "ignition", so that the combustion reaction is already occurring at the beginning of the calculation. The working conditions solved in this paper are shown in Table 2.

Table 2 Initial condition set

Serial number	Equivalent ratio	Velocity (m/s)
1	0.35	0.85
2	0.45	0.85
3	0.55	0.85
4	0.65	0.85
5	0.75	0.85
6	0.85	0.85
7	0.65	0.65
8	0.65	0.75
9	0.65	0.95
10	0.65	1.05

According to the Settings in Table 2, the combustion characteristics of the new porous medium burner and the emission of main pollutant NOx at different equivalent ratios and inlet flow rates are explored.

Based on the numerical simulation results, the comparison and verification with the double-porous media burners in the existing literature [14] are carried out. Under the condition that other conditions remain unchanged, the change law between the maximum temperature and equivalent ratio in the burner is shown in Figure 5 below.

2.6 Model Verification

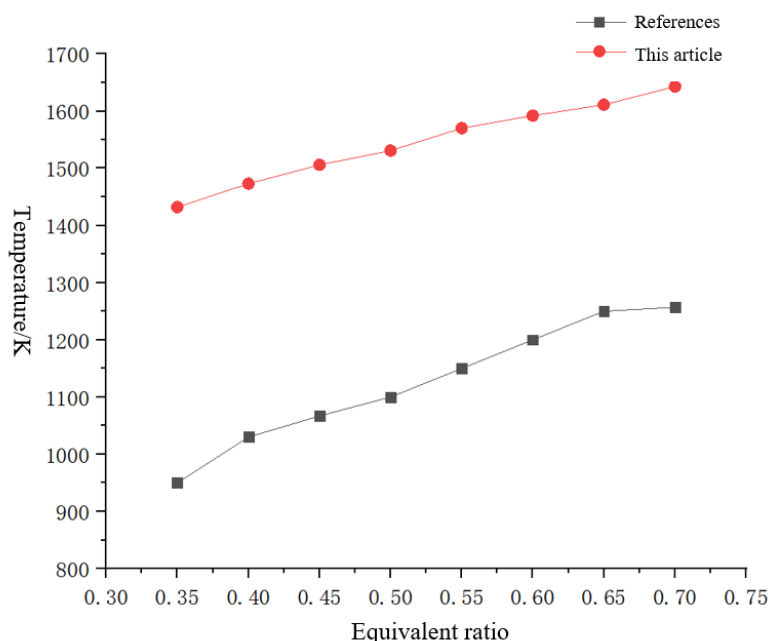


Figure 5 The relationship between combustion temperature and equivalent ratio

As can be seen from Figure 4, the burner model established in this paper is basically the same as the simulation results in the existing literature [14]. The maximum slope error between each section of the two curves is less than 8%, which proves that the accuracy of the numerical simulation model established in this paper is in line with the error range.

3. Combustion characteristics analysis of new porous medium burner

3.1 Influence of premixed gas equivalent ratio

Figure 6 shows the axial distribution of temperature calculated in working conditions 1-5 in Table 2.

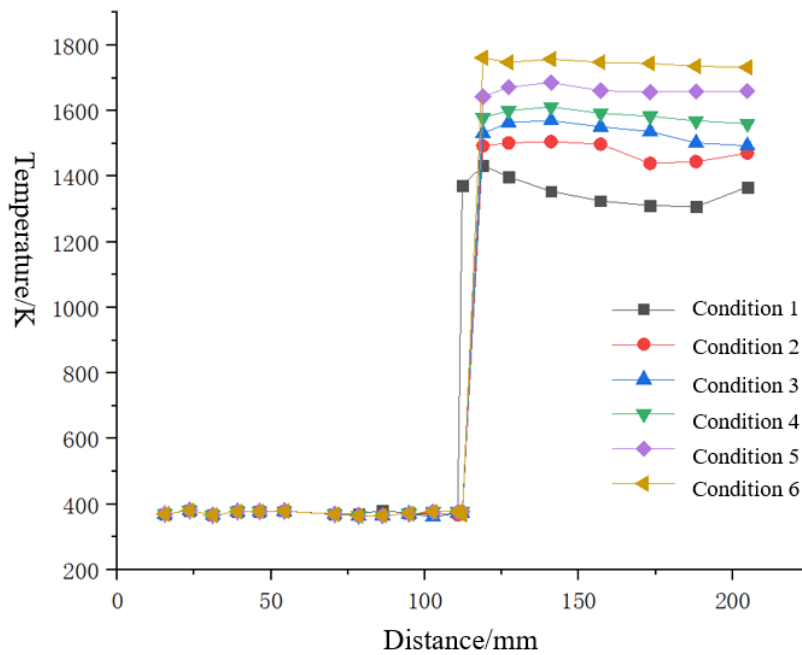


Figure 6 Axial temperature distribution at different equivalent ratios

As can be seen from Figure 5, the change of burner temperature in the small hole medium region (0-120mm) is not obvious, that is, the combustion reaction in this region has not fully developed, indicating that the pre-mixed gas starts to burn in large quantity near the porous medium intersection interface (x-y/mm), and the flame surface is formed in the large hole medium region as the combustion region. When the inlet flow rate is constant, the temperature of the burner near the interface of porous media increases rapidly with the increase of equivalent ratio, and the equivalent ratio is 0.85 when the highest temperature is 1657K. In addition, with the increase of equivalent ratio, there is a slight forward shift in the temperature mutation during ignition, indicating that pre-mixed gas with relatively large equivalent is more likely to ignite after heat exchange when it does not enter

the combustion zone.

3.2 Influence of premixed gas inlet velocity

In order to accurately analyze the influence of inlet velocity change on combustion state, it is necessary to ensure the same equivalent ratio and constantly change the flow rate of mixture. Therefore, different flow rates with equivalent ratio of 0.65 are selected for simulation in this paper, that is, conditions 7-10 and 4 in Table 2 are used to ensure that the flow rate ranges from 0.65 to 1.05m/s and is solved with a span of 0.1m/s. The calculated maximum temperature curve is shown in Figure 7, and the cloud image at the highest temperature is shown in Figure 8.

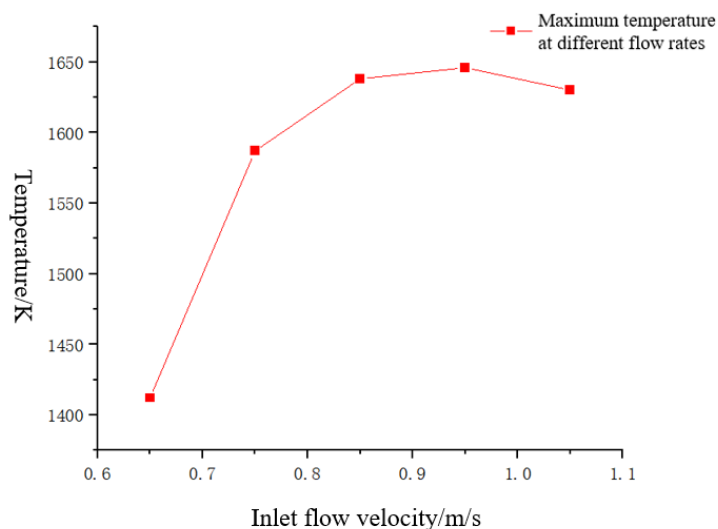
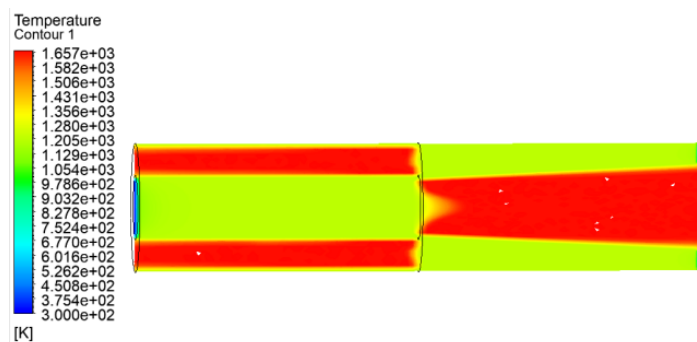


Figure 7 The highest temperature of burner under different flow rate



Figureure 8 Burner temperature nephogram

As can be seen from Figureure. 7 and Figureure. 8, in the flow rate range of this study, the outlet temperature ranges from 1432K to 1657K, which is acceptable considering the high temperature resistance of porous media in practical industrial applications. At the same time, in the flow rate range of 0.65m/s-1.05m/s, the temperature peak value of the improved porous medium burner is always higher than that of the original burner. The reason is that the inclined structure makes the gas flow in the porous medium strengthen, the combustion area increases, and the flame width is higher when ignition at the same position in terms of the ignition area. As far as the preheating zone is concerned, the inclined structure makes the lower gas temperature in the preheating zone higher and the upper gas lower, and the hot gas moves upward after being heated, thus promoting the full preheating of the gas in the preheating zone.

3.3 NOx emission characteristics of new burners

The combustion of hydrocarbon fuel inevitably produces toxic gases, which are directly discharged into the atmosphere, not only affecting the living environment, but also seriously endangering human health, among which the main pollutants are CO and NO. Therefore, how to reduce the emission of CO, NO and other toxic gases

during combustion is also one of the hot research issues.

The combustion characteristics of ethylene are closely related to its concentration, and the equivalent ratio determines the concentration of ethylene in the airflow. Higher ethylene concentration makes it easier for the mixture to achieve combustion conditions and generate higher heat in subsequent combustion, while the flow rate will affect the temperature field and mass fraction distribution of each component in the combustion chamber, thus changing the combustion characteristics of ethylene and pollutant generation [16]. Therefore, it is of great significance to investigate the combustion characteristics of ethylene at different flow rates and equivalent ratios. When the combustion reaction occurs, the nitrogen components in the air and fuel are decomposed by heat, and toxic nitrogen oxides are generated under the oxidizing conditions of combustion. The components are mainly NO and NO₂, collectively known as NO_x. The emission of nitrogen oxides is harmful to human body and nature, so all countries have strict regulations on its emission [17].

In this paper, given the inlet flow rate of 0.65m/s, the equivalent ratio of pre-mixed gas is changed to explore the CO and Nitrogen oxide emission at 0.35, 0.45, 0.55, 0.65, 0.75, 0.85 equivalent ratio. FIG. 9 shows the concentration curves of CO and NO_x along the axial direction under different equivalent ratios.

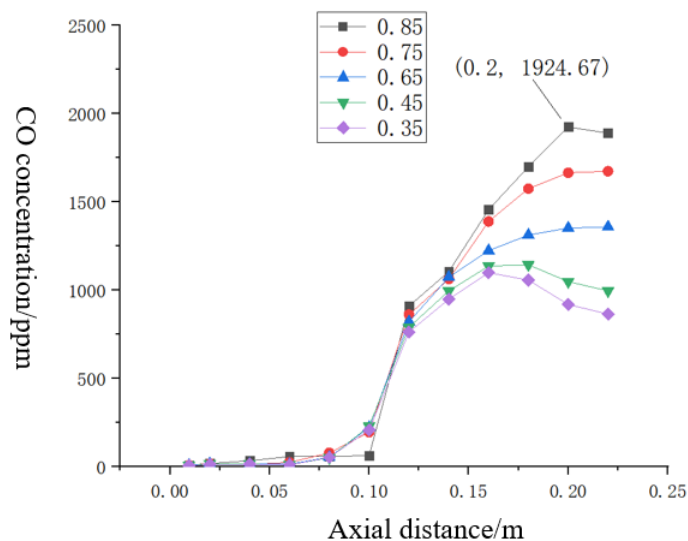


Figure 9 CO concentration curve

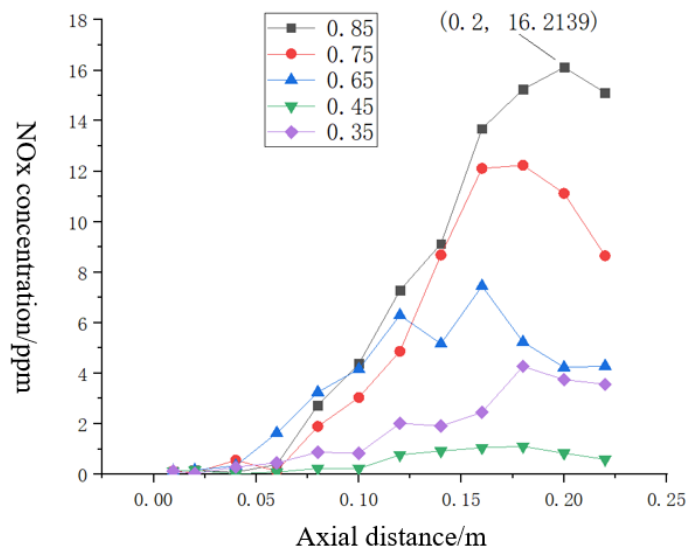


Figure 10 NOx concentration curve

Through the comparative analysis of FIG. 9 and FIG. 10, it is found that the relationship between equivalent ratio and NOx emission does not follow a strict consistency relationship when the ethylene content is constant. Among them, when the equivalent ratio is 0.45, the NOx emission is significantly lower than that of 0.35, indicating that selecting the appropriate equivalent ratio to make the combustion fully can effectively inhibit the NOx emission. But on the whole, NOx emissions will show an upward trend with the increase of equivalent ratio, which is because the increase of equivalent ratio will lead to the increase of combustible gas flow, combustion reaction is more incomplete, and the temperature is higher when the equivalent is larger, more conducive to the production of pollutants. In terms of pollutant emissions, CO emissions decreased from 3100ppm to 1924.67ppm before and after the improvement, a decrease of 37.9%. As for NO emission, it can be seen from the slopes of each broken line in Figure 9 that NO emission gradually increases with the increase of equivalent ratio. This is because the temperature peak value is higher when the equivalent ratio is high, which accelerates the reaction rate of CN-N2. Rapid type NO was produced, and the emission of NO increased from 12.14ppm to 16.21ppm, which was caused by higher combustion temperature after the structural improvement. Overall, the emission of NO was still in a low state.

4. Conclusion

In this paper, a new type of porous media burner is designed, a numerical analysis model is established according to the assumptions, and compared with the test data in literature [15], the accuracy of the established model is verified by trend analysis. Based on this model, combustion characteristics and pollutant emission characteristics of new burners at different flow rates and equivalent ratios are studied, and the following conclusions are obtained:

(1) Under the condition that the inlet velocity of premixed gas is unchanged, only the equivalent ratio of the inlet is changed, and the gas heated in the preheating

zone of the new burner accelerates the full preheating of the gas and achieves the purpose of full preheating; The inclined structure in the combustion zone further enlarges the combustion zone and improves the flame width. Compared with the original structure, the maximum combustion temperature can reach 1757K when the equivalent ratio is 0.85, and the combustion is more full.

(2) When the equivalent ratio is unchanged, the maximum temperature increases rapidly with the increase of the inlet flow velocity within the range of 0.65-0.85m/s. This is because in the process of flame propagation, the direction of combustion wave propagation is opposite to the direction of premixed gas flow, and the increase of premixed gas flow velocity will cause the flame to burn slowly. More fuel can be burned in a unit of time to release more heat value, but also can better preheat the upstream premixed gas. When the flow rate was 0.85m/s, the temperature rise effect increased slowly. Therefore, under this condition, 0.85m/s can be set as the inlet velocity of combustion, so as to facilitate the full progress of combustion.

(3) The emission characteristics of pollutants in the new porous medium burner were improved. Under the same conditions as the literature flow rate and enriched combustion (equivalent ratio of 0.85), the CO emission decreased by 37.9%, and the NOx emission only increased by 4.07ppm, which showed that the secondary pollution to the environment was reduced while the combustion efficiency was improved.

Acknowledgements

This work has been supported by the project of Supporting Enterprise Technological Innovation and Development in Hubei Province. (Project No. :2021BAB112)

This work is supported by the 2022 Central Guidance Local Science and Technology Development Fund project. (Project No. :2022BGE005)

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