

## Article

# Numerical Simulation of Catalytic Methane Combustion in $\text{Al}_2\text{O}_3$ Directional Nanotubes Modified by Pt and Pd Catalyst

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**Abstract:** “Blind holes” are the main reasons for the reduced performance of microgas sensor carriers. To improve the “blind hole” of catalytic combustion methane sensors and therefore, their thermal stability, this study presents a numerical simulation of the catalytic combustion in an  $\text{Al}_2\text{O}_3$  - oriented ceramic array involving porous microthermal plates. A three-visualization model of the sensor is established using the FLUENT software, and the simulation results are systematically analyzed based on the dynamics and thermodynamic mechanism of the microgas sensor. The results show that the regularity of the surface reaction presents a circular distribution, with the center line of the channel serving as the axis symmetry. The total reaction velocity in the array hole increases gradually from the inlet to the outlet. The flow velocity at the inlet should be controlled at more than  $1 \times 10^{-8}$  m/s, which is more accurate compared with the concept of “uniform velocity” in previous studies. The optimum pore size at the inlet should be 150 nm, and the inner pore size of the wall should be slightly higher than 300 nm, which is a more careful division compared with previous pore-size studies. The efficient reaction position is from the inlet to the quarter of the hole. The simulation results make up for the deficiencies in the analysis of the process parameters of the methane sensor carrier array hole and the internal reaction change process, as well as provide innovative comments on the sensor structure design. Through digital simulations, the limitations associated with the experiments can be avoided, the theoretical study can be improved, theoretical support can be provided for experiments related to the improvement of thermal stability, the predictability of experiments can be improved, and the feasibility of the research proposal can be verified. These steps are important for the improvement of the “blind hole” problem of catalytic combustion methane sensors.

**Keywords:** blind hole; numerical simulation of catalytic combustion; sensor model; thermodynamic mechanism; flow velocity; hole size



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## 1. Introduction

Large amounts of gas are generated during the coal-mining process. Its main component is methane (about 83–89%), which is flammable and explosive, and its explosion range is 5–16% [1–3] of the volume fraction. Therefore, it is particularly important to achieve accurate monitoring of underground methane. In recent years, with rapid industrialization, many methane sensors have emerged, which can be divided into infrared spectral, semiconductor, ultrasonic, and catalytic combustion according to the different detection principles. Compared with other types of sensors, the catalytic combustion type exhibits high sensitivity, fast response time, stable performance, and low-power consumption, has a simple production process, and has an inexpensive nature. At present, catalytic combustion technology is widely used in coal-mine-networking methane sensors and is the most economical and effective among other options [4], making it suitable for the development needs of the Internet of Things in the construction of smart mines. Therefore, it is necessary

to perform a system simulation of catalytic combustion methane sensors to improve their local performance. The sensor structure can also be improved, and external factors can be adjusted to enhance their overall performance.

Based on the different structures of catalytic combustion methane sensors, it is mainly divided into two structures: traditional pellet-shaped and silicon-based planar array plates. The sensor carrier is prepared, and the catalyst is loaded by impregnating the same volume of catalyst and promoter into  $\text{Al}_2\text{O}_3$  powder [5]. Although it has the advantages of a large specific surface area and simple process [6], its “blind hole” makes methane burn on the surface of the sensor, while the limited diffusion of reactants affects the activity of the catalyst and even deactivates, resulting in the decrease of the sensor’s stability, performance, and detection accuracy [7,8]. Yang et al. [9] prepared palladium and multiwalled carbon nanotube (MWNT) composites using the simple method of reducing  $\text{NaBH}$  aqueous mixture, thereby improving the detection ability of the sensor for methane at room temperature. Roy [10] deposited carbon nanotubes (CNTs) by electrodeposition technology to reduce their hole concentration and increase the resistivity of the manufactured  $\text{CH}_4$  sensor. Chen et al. [11] developed lithium-ion-doped CNTs as sensing elements to detect and estimate methane, resulting in sensors with a maximum sensitivity at 14 ppm of ~5.500%. Zhang et al. [12] used MWNTs combined with carrier modification technology to produce a fast-response thermal conductivity gas sensor, thereby improving the response speed of the methane sensor. Forough Kalantari Fotooh [13] modified single-walled CNTs with transition metals (Fe, Ni, and Pd), enhanced the adsorption capacity of methane, and improved the sensitivity and selectivity of the sensor.

Additionally, microheating plates have also been developed. For example, Roslyakov et al. [14] developed a microheating plate catalytic methane sensor based on porous anodic alumina and achieved a sensor response value of ~15 mV/vol. Tang et al. [15] found that using insulating thermal conductive film can greatly improve the temperature under the same voltage by comparing three types of microheating plates with different structures. Kulhari [16] and Kharbanda et al. [17] arranged the heating resistor and interdigital electrode on the front and back of the LTCC ceramic plate and found that the sensor has good thermal stability. Yuan et al. [18] used a silicon-based microelectromechanical system (MEMS) to conduct microheating plate processing and electrical connection according to the parameters optimized using the finite element method. They also designed a microheating plate with low-power consumption. The abovementioned studies improved the sensitivity and detection accuracy of methane sensors at varying degrees. However, whether the introduction of carbon nanotube-modified carriers or the direct use of porous ceramic microhotplates can form the structure of noble metal catalysts supported by nanopores [19,20], resulting in the so-called “blind holes”, has yet to be fully investigated. Furthermore, the problem involving blind holes in sensors has not been effectively solved so far. Therefore, overcoming the “blind hole” of the traditional “pellet” methane sensor powder ball and the silicon-based planar microhotplate carrier as well as improving the thermal stability of the carrier are the scientific problems that should be solved urgently by researching catalytic gas sensors.

In this study, the directional ceramic array hole microhotplate is taken as an example for further examination. By building a physical model of the sensor, combined with the basic theory of thermal analysis of microgas sensors and the process parameters of sensitive components, the two catalytic combustion modes occurring during the operation of the methane sensor are numerically simulated. Furthermore, while studying the reaction speed, temperature field distribution, and species mass fraction distribution in the channel during operation, variables, such as reactant concentration and hole size, are considered in the comprehensive analysis. Furthermore, the thermodynamic mechanism of the catalytic combustion methane sensor with oriented ceramic array pore microthermal plate is revealed, the catalytic combustion characteristics of the micropore are explored, and the optimal size of the array pore is determined in a breakthrough. Finally, a new pore structure is designed,

and the optimal reaction interval of the gas inside the pore is determined along with the minimum velocity of methane entering the pore.

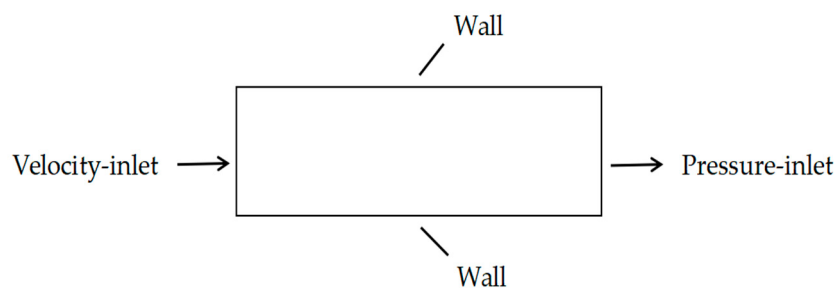
The innovative application of numerical simulations deepens the theoretical study and complements and explains the physical processes and phenomena that cannot be observed experimentally. The results obtained have made a breakthrough in sensor microstructure system fabrication processes and materials, improved the working performance of sensitive elements, and provided the experimental basis and data support to improve the thermal stability of catalytic combustion methane sensors. Furthermore, the results reduced the experimental trial and error rate, improved experimental efficiency, and managed the blindness issue of ceramic array pore microthermal plate carriers. Finally, they also resolved the blind hole problem of ceramic array pore microthermal plate carrier, enhanced the overall performance of the sensor, provided experimental basis and reasonable scheme design for the accurate use of the sensor in the future, and improved the practical application value of the sensor.

## 2. Materials and Methods

After establishing a three-dimensional (3D) visualization model of the sensor, the model is solved and analyzed through the kinetic and thermodynamic mechanisms of microgas in the array pores using molecular dynamics simulation methods and the basic theory of thermal analysis. Moreover, the boundary conditions are set by considering the sensitive element process parameters, reactant ratios, and other conditions. The thermal analysis of the microgas sensor involves the standard  $\kappa - \varepsilon$  turbulence model, component transport model, and thermal analysis model. The FLUENT software is used for the simulation, which contains the functional modules corresponding to the above three models and can perfectly fit the changing states of the substances and the environment during methane combustion. The basic theories involved in the three models are explained in the following subsections.

### 2.1. Physical Model and Working Mechanism

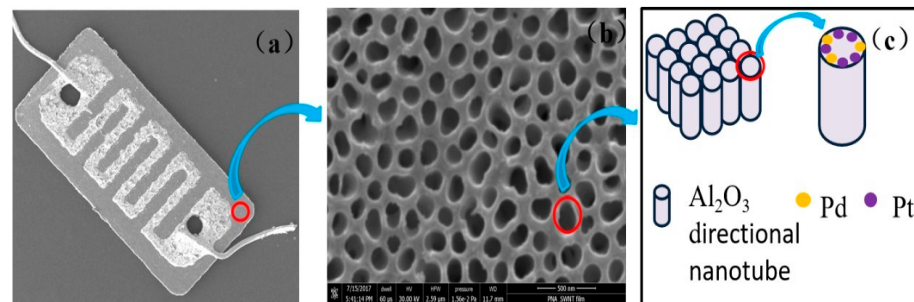
As mentioned previously, the FLUENT fluid dynamics software is used for simulation. The two-dimensional (2D) model is shown in Figure 1, including the annular wall and the sensor inlet and outlet.



**Figure 1.** Microporous reaction model.

The physical object and 3D model of the sensor are shown in Figure 2 [21]. The main supporting component of the gas sensor is the microhotplate, as shown in Figure 2a. The Pt resistance is screen printed on the porous  $\text{Al}_2\text{O}_3$  substrate. The detection mechanism is that once the methane gas is mixed with oxygen in the air, it penetrates the porous film, and a catalytic combustion reaction occurs [22]. The reaction heat heats the Pt resistance [23], causing the resistance value to change, after which it outputs a stable voltage signal that is proportional to the gas concentration [24]. As shown in Figure 2b, the substrate is covered with micropores, which is the main reason for methane combustion. The inner walls of the pore are modified with catalysts, such as platinum and palladium, to form a spill-over effect [25] between them and  $\text{Al}_2\text{O}_3$ ; here, the wall surface is also a reaction occasion.

Figure 2c presents a 3D model of the oriented ceramic array hole, which visually shows its basic structure and the distribution of various substances.



**Figure 2.** Oriented ceramic array hole microhotplate: (a) the microhotplate; (b) array hole; (c) 3D model of the oriented ceramic array hole.

## 2.2. Fluid Turbulence Model

The heat generated due to gas combustion will heat the gas. The heated gas flow is turbulent; therefore, it should be described using turbulence equations, which involve three partial differential equations [26,27].

(1) Mass conservation equation:

$$\frac{\partial \bar{u}}{\partial x} + \frac{\partial \bar{v}}{\partial y} + \frac{\partial \bar{w}}{\partial z} = 0. \quad (1)$$

Note that the equation is mean, and the speed is time-averaged speed  $\bar{u}, \bar{v}, \bar{w}$ .

(2) Momentum conservation equation:

$$\begin{cases} \rho \left[ \frac{\partial \bar{u}}{\partial t} + \frac{\partial(\bar{u}\bar{u})}{\partial x} + \frac{\partial(\bar{u}\bar{v})}{\partial y} + \frac{\partial(\bar{u}\bar{w})}{\partial z} \right] = -\frac{\partial \bar{p}}{\partial x} + \nu \nabla^2 \bar{u} + \left[ \frac{\partial(-\rho \bar{u}'u')}{\partial x} + \frac{\partial(-\rho \bar{u}'v')}{\partial x} + \frac{\partial(-\rho \bar{u}'w')}{\partial x} \right] \\ \rho \left[ \frac{\partial \bar{v}}{\partial t} + \frac{\partial(\bar{v}\bar{u})}{\partial x} + \frac{\partial(\bar{v}\bar{v})}{\partial y} + \frac{\partial(\bar{v}\bar{w})}{\partial z} \right] = -\frac{\partial \bar{p}}{\partial y} + \nu \nabla^2 \bar{v} + \left[ \frac{\partial(-\rho \bar{v}'u')}{\partial y} + \frac{\partial(-\rho \bar{v}'v')}{\partial y} + \frac{\partial(-\rho \bar{v}'w')}{\partial y} \right] \\ \rho \left[ \frac{\partial \bar{w}}{\partial t} + \frac{\partial(\bar{w}\bar{u})}{\partial x} + \frac{\partial(\bar{w}\bar{v})}{\partial y} + \frac{\partial(\bar{w}\bar{w})}{\partial z} \right] = -\frac{\partial \bar{p}}{\partial z} + \nu \nabla^2 \bar{w} + \left[ \frac{\partial(-\rho \bar{w}'u')}{\partial z} + \frac{\partial(-\rho \bar{w}'v')}{\partial z} + \frac{\partial(-\rho \bar{w}'w')}{\partial z} \right] \end{cases}. \quad (2)$$

Note that the equation contains the Reynolds stress caused by the pulsating velocity (i.e., the third term on the right side of the equal sign). Thus, to make the equation closed, a new equation must be introduced. This study uses the standard  $\kappa - \varepsilon$  model, which defines the turbulent kinetic energy,  $\kappa$ , and turbulent kinetic energy dissipation rate,  $\varepsilon$ , as follows:

$$\varepsilon = \frac{\mu}{\rho} \overline{\left( \frac{\partial u'_i}{\partial x_k} \right) \left( \frac{\partial u'_i}{\partial x_k} \right)}, \quad (3)$$

where  $\mu$  is the viscosity of gas, and  $\mu_t$  is expressed as a function of  $\kappa$  and  $\varepsilon$ , as follows:

$$\mu_t = \rho C_\mu \frac{\kappa^2}{\varepsilon}, \quad (4)$$

The transport equations corresponding to turbulent kinetic energy,  $\kappa$ , and energy dissipation rate,  $\varepsilon$ , are as follows:

$$\frac{\partial(\rho \bar{\kappa})}{\partial t} + \frac{\partial(\rho \bar{\kappa} u_i)}{\partial x_i} = \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{\sigma_\kappa} \right) \frac{\partial \bar{\kappa}}{\partial x_j} \right] + G_\kappa + G_b - \rho \bar{\varepsilon} - Y_M + S_\kappa, \quad (5)$$

$$\frac{\partial(\rho \bar{\varepsilon})}{\partial t} + \frac{\partial(\rho \bar{\varepsilon} u_i)}{\partial x_i} = \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{\sigma_\varepsilon} \right) \frac{\partial \bar{\varepsilon}}{\partial x_j} \right] + C_{1\varepsilon} \frac{\bar{\varepsilon}}{\kappa} (G_\kappa + C_{3\varepsilon} G_b) - C_{2\varepsilon} \rho \frac{\bar{\varepsilon}^2}{\kappa} + S_\varepsilon, \quad (6)$$

where  $G_\kappa$ —generating term of turbulent kinetic energy,  $\kappa$ , due to mean velocity gradient,

$$G_\kappa = \mu_t \left( \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) \frac{\partial \bar{u}_i}{\partial x_j};$$

$G_b$ —generating term of turbulent kinetic energy,  $\kappa$ , due to buoyancy,  $G_b = \beta g_i \frac{\mu_t}{Pr_t} \frac{\partial T}{\partial x_i}$ ;

$Y_M$ —contribution of pulsation expansion in compressible turbulence;

$C_{1\varepsilon}$ ,  $C_{2\varepsilon}$ ,  $C_{3\varepsilon}$ —empirical constant;

$\sigma_k$ ,  $\sigma_\varepsilon$ —Prandtl number corresponding to turbulent kinetic energy and dissipation rate  $\kappa$ ,  $\varepsilon$ ;

$S_k$ ,  $S_\varepsilon$ —source term defined by the user according to the calculation condition;

$Pr_t$ —turbulent Prandtl number is 0.85 in this model;

$g_i$ —gravity acceleration component in the  $i$  direction; and

$\beta$ —thermal expansion coefficient,  $\beta = -\frac{1}{\rho} \frac{\partial \rho}{\partial T}$ .

### (3) Energy-conservation equation:

Given that gas combustion involves energy conversion and temperature change, the energy equation must be included as follows:

$$\frac{\partial(\rho T)}{\partial t} + \nabla \cdot (\rho \bar{u}_i T) = \nabla \cdot \left[ \left( \frac{\mu}{Pr} + \frac{\mu_t}{\sigma_T} \right) \nabla T \right], \quad (7)$$

where  $i = x, y$ , and  $z$ , and  $T$  is the temperature.

### 2.3. Chemical Reaction Model

The combustion reaction is essentially a chemical reaction; hence, in addition to the above equations, the chemical reaction equation must be included. As the fluid flow is disordered during combustion, the reaction rate is controlled by mixed turbulence. Additionally, before the measured gas methane enters the porous medium or micropore, it can be considered that it has been fully mixed with oxygen. Therefore, the eddy dissipation model is used in this study. The FLUENT software provides this model. In this model, the production rate,  $R_{i,r}$ , of substance  $i$  in the  $r$ th reaction can be determined by a smaller one of the following equations:

$$R_{i,r} = v'_{i,r} M_{w,i} A \rho \frac{\epsilon}{k} \min \frac{Y_R}{v'_{R,r} M_{w,R}}, \quad (8)$$

$$R_{i,r} = v'_{i,r} M_{w,i} A B \rho \frac{\epsilon}{k} \frac{\sum_p Y_p}{\sum_j^N v''_{j,r} M_{w,j}}, \quad (9)$$

In Equations (8) and (9) [28], the chemical reaction rate is controlled by the large eddy mixing time scale  $\frac{k}{\epsilon}$ . As long as the turbulence is  $\frac{k}{\epsilon} > 0$ , combustion can be conducted without the ignition source.

### 2.4. Chemical Reaction Mechanism

#### (1) Body-reaction mechanism [29]

The total reaction equation of methane and air is given by:



In fact, it includes many elementary reactions. For simplification, a five-step reaction mechanism is adopted, as shown in Table 1.

## (2) Wall reaction mechanism [30]

**Table 1.** Body reaction mechanism.

| Reaction Serial Number | Response Equation                                                  | Pre-Exponential Factor (A,m.mol.s) | Temperature Index ( $\beta$ ) | Activation Energy $E_a$ (J/mol) | Reaction Rate Index                              |
|------------------------|--------------------------------------------------------------------|------------------------------------|-------------------------------|---------------------------------|--------------------------------------------------|
| 1                      | $\text{CH}_4 + 1.5\text{O}_2 \geq \text{CO} + 2\text{H}_2\text{O}$ | $1.6596 \times 10^{15}$            | 0.000                         | $1.72 \times 10^8$              | FORD/CH <sub>4</sub> 1.46/O <sub>2</sub> 0.5217/ |
| 2                      | $\text{CO} + 0.5\text{O}_2 \geq \text{CO}_2$                       | $7.9799 \times 10^{14}$            | 0.000                         | $9.654 \times 10^7$             | FORD/CO 1.6904/O <sub>2</sub> 1.57/              |
| 3                      | $\text{CO}_2 \geq \text{CO} + 0.5\text{O}_2$                       | $2.2336 \times 10^{14}$            | 0.000                         | $5.1774 \times 10^8$            | $K = AT^\beta \exp(E_a/kT)$                      |
| 4                      | $\text{N}_2 + \text{O}_2 \geq 2\text{NO}$                          | $8.8308 \times 10^{23}$            | 0.000                         | $4.4366 \times 10^8$            |                                                  |
| 5                      | $\text{N}_2 + \text{O}_2 \geq 2\text{NO}$                          | $9.2683 \times 10^{14}$            | −0.500                        | $5.727 \times 10^8$             |                                                  |

The wall reaction adopts a 23-step mechanism, as shown in Table 2.

**Table 2.** Wall reaction mechanism.

| Reaction Serial Number | Response Equation                                                               | Pre-Exponential Factor (m.mol.s) | Cover Degree | Temperature Index   | Activation Energy (J/mol) | Speed Index     |
|------------------------|---------------------------------------------------------------------------------|----------------------------------|--------------|---------------------|---------------------------|-----------------|
| 1                      | $\text{O}_2 + 2\text{PT(S)} \geq 2\text{O(S)}$                                  | -                                | 0.003        | 0                   | 0                         |                 |
| 2                      | $\text{CH}_4 + 2\text{PT(S)} \geq \text{CH}_3\text{(S)} + \text{H(S)}$          | -                                | 0.15         | $9.654 \times 10^7$ | 28,000.00                 | FORD/PT(S) 2.3/ |
| 3                      | $\text{CH}_4 + \text{O(S)} \geq \text{CH}_3\text{(S)} + \text{OH(S)}$           | -                                | 0.43         | 0                   | 59,200.00                 |                 |
| 4                      | $\text{CO} + \text{PT(S)} \geq \text{CO(S)}$                                    | -                                | 0.840        | 0                   | 0                         | FORD/PT(S) 2/   |
| 5                      | $\text{H}_2 + 2\text{PT(S)} \geq 2\text{H(S)}$                                  | -                                | 0.046        | 0.00                | 0.00                      | FORD/PT(S) 1.0/ |
| 6                      | $\text{OH} + \text{PT(S)} \geq \text{OH(S)}$                                    | -                                | 1.00         | 0.0                 | 0.0                       |                 |
| 7                      | $\text{H}_2\text{O} + \text{PT(S)} \geq \text{H}_2\text{O(S)}$                  | -                                | 0.5          | 0.0                 | 0.0                       |                 |
| 8                      | $\text{CH}_3\text{(S)} + \text{PT(S)} \geq \text{CH}_2\text{(S)} + \text{H(S)}$ | $1.0 \times 10^{21}$             | -            | 0.00                | 20,000.0                  |                 |
| 9                      | $\text{CH}_2\text{(S)} + \text{PT(S)} \geq \text{CH(S)} + \text{H(S)}$          | $1.0 \times 10^{21}$             | -            | 0.00                | 20,000.0                  |                 |
| 10                     | $\text{CH(S)} + \text{PT(S)} \geq \text{C(S)} + \text{H(S)}$                    | $1.0 \times 10^{21}$             | -            | 0.00                | 20,000.0                  |                 |
| 11                     | $\text{H(S)} + \text{O(S)} = \text{OH} + 2\text{PT(S)}$                         | $1.0 \times 10^{20}$             | -            | 0.00                | 10,500.0                  |                 |
| 12                     | $\text{OH(S)} = \text{H(S)} + \text{O(S)}$                                      | $1.0 \times 10^{12}$             | -            | 0.00                | 20,800.0                  |                 |
| 13                     | $\text{H(S)} + \text{OH(S)} = \text{H}_2\text{O(S)}$                            | $1.0 \times 10^{21}$             | -            | 0.00                | 62,500.0                  |                 |
| 14                     | $\text{OH(S)} + \text{OH(S)} = \text{H}_2\text{O(S)} + \text{O(S)}$             | $1.0 \times 10^{20}$             | -            | 0.00                | 51,250.0                  |                 |
| 15                     | $\text{H}_2\text{O(S)} \geq \text{H(S)} + \text{OH(S)}$                         | $1.0 \times 10^{13}$             | -            | 0.00                | 51,200.0                  |                 |
| 16                     | $\text{C(S)} + \text{O(S)} \geq \text{CO(S)}$                                   | $5.0 \times 10^{20}$             | -            | 0.00                | 62,500.0                  |                 |
| 17                     | $\text{CO(S)} \geq \text{C(S)} + \text{O(S)}$                                   | $1.0 \times 10^{13}$             | -            | 0.00                | 156,500.0                 |                 |
| 18                     | $\text{CO(S)} + \text{O(S)} \geq \text{CO} + \text{PT(S)}$                      | $4.0 \times 10^{20}$             | -            | 0.00                | 49,140.0                  |                 |
| 19                     | $2\text{O(S)} \geq \text{O}_2 + 2\text{PT(S)}$                                  | $1.0 \times 10^{21}$             | -            | 0.00                | 21,600.0                  |                 |
| 20                     | $\text{CO(S)} \geq \text{CO} + 2\text{PT(S)}$                                   | $8.5 \times 10^{12}$             | -            | 0.00                | 152,500.0                 |                 |
| 21                     | $2\text{H(S)} \geq \text{H}_2 + 2\text{PT(S)}$                                  | $5.0 \times 10^{20}$             | -            | 0.00                | 67,400.0                  |                 |
| 22                     | $\text{OH(S)} \geq \text{OH} + \text{PT(S)}$                                    | $1.5 \times 10^{13}$             | -            | 0.00                | 192,800.0                 |                 |
| 23                     | $\text{H}_2\text{O(S)} \geq \text{H}_2\text{O} + \text{PT(S)}$                  | $1.0 \times 10^{13}$             | -            | 0.00                | 45,000.0                  |                 |

### 3. Results and Discussion

#### 3.1. Analysis of the Microporous Body-Reaction Combustion Simulation

As methane and air mainly burn in micropores [31], the gas in micropores is taken as the simulation object and discretized. Then, the above sensor physical model, thermal analysis theoretical model, and reaction mechanism are loaded into FLUENT, after which certain boundary conditions are applied for calculation. Based on this data, the volume

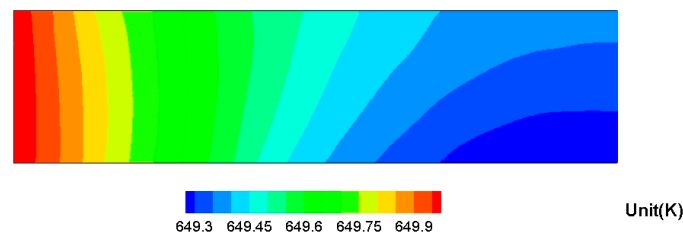
reaction of methane in micropores is simulated. The boundary conditions setting is shown in Table 3.

**Table 3.** Boundary conditions setting.

| Inlet Velocity (m/s)    | Equivalence Ratio | CH <sub>4</sub> Mass Fraction (%) | O <sub>2</sub> Mass Fraction (%) | Pore Size (nm) | Wall Shear | Outlet (atm) |
|-------------------------|-------------------|-----------------------------------|----------------------------------|----------------|------------|--------------|
| (1) $6 \times 10^{-8}$  | (I) 0.3           | 0.016875                          | 0.225                            | (a) 60         | Adiabatic  | 1            |
| (2) $1 \times 10^{-7}$  | (II) 0.6          | 0.034                             | 0.225                            | (b) 150        | Adiabatic  | 1            |
| (3) $13 \times 10^{-8}$ | (III) 1           | 0.05625                           | 0.225                            | (c) 300        | Adiabatic  | 1            |

### 3.1.1. Body-Reaction Temperature Field

The simulation results of the combustion temperature field in the micropore are shown in Figure 3. For the bulk reaction, combustion mainly occurs near the entrance, and the temperature in the orifice is the highest, which exhibits a decreasing trend along the depth of the hole. Furthermore, the temperature inside the hole is slightly lower; however, because the size is nanoscale, the overall temperature difference is not large.

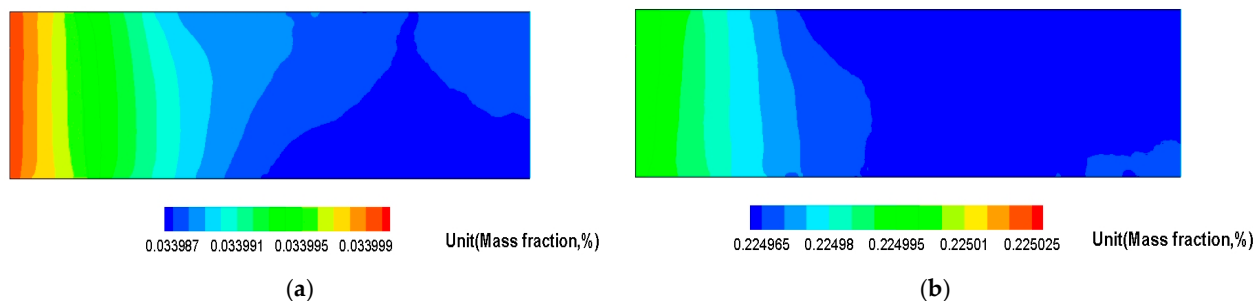


**Figure 3.** Microporous body reaction temperature field.

### 3.1.2. Species Mass Fraction

#### (1) Distribution of the reactant mass fraction

Figure 4a shows the distribution of the methane mass fraction. It can be seen that the concentration is high at the inlet. After the reaction, the concentration gradually decreases along the hole depth direction, while the methane mass fraction at the same hole depth section near the orifice shows a uniform distribution. Figure 4b presents the oxygen mass fraction distribution map. According to the bulk reaction mechanism, methane and oxygen participate in the reaction simultaneously; therefore, the distribution of oxygen is similar to that of methane. Methane combustion requires more oxygen than its own volume, and the same gradient mass fraction of oxygen is lower than methane.

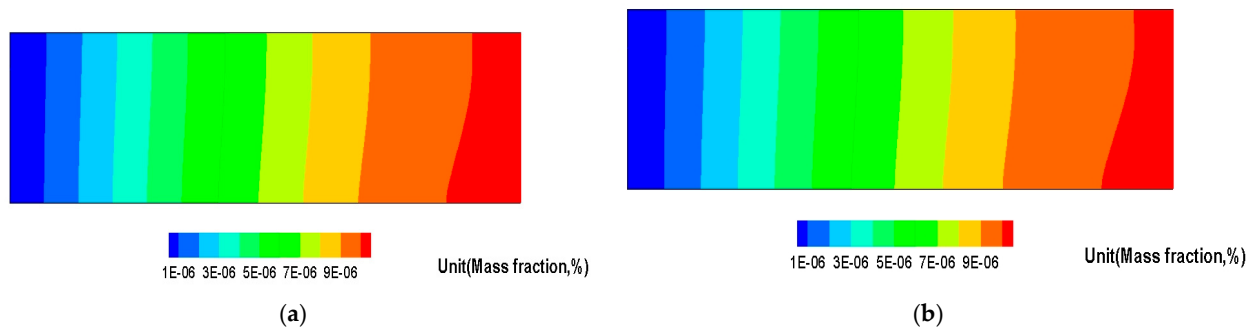


**Figure 4.** Distribution of reactant mass fraction: (a) methane mass fraction distribution; (b) oxygen mass fraction distribution.

#### (2) Distribution of product mass fraction

After the reaction, the obtained products are mainly H<sub>2</sub>O and CO<sub>2</sub>, as shown in Figure 5. Figure 5a,b present the H<sub>2</sub>O concentration distribution map and CO<sub>2</sub> concentra-

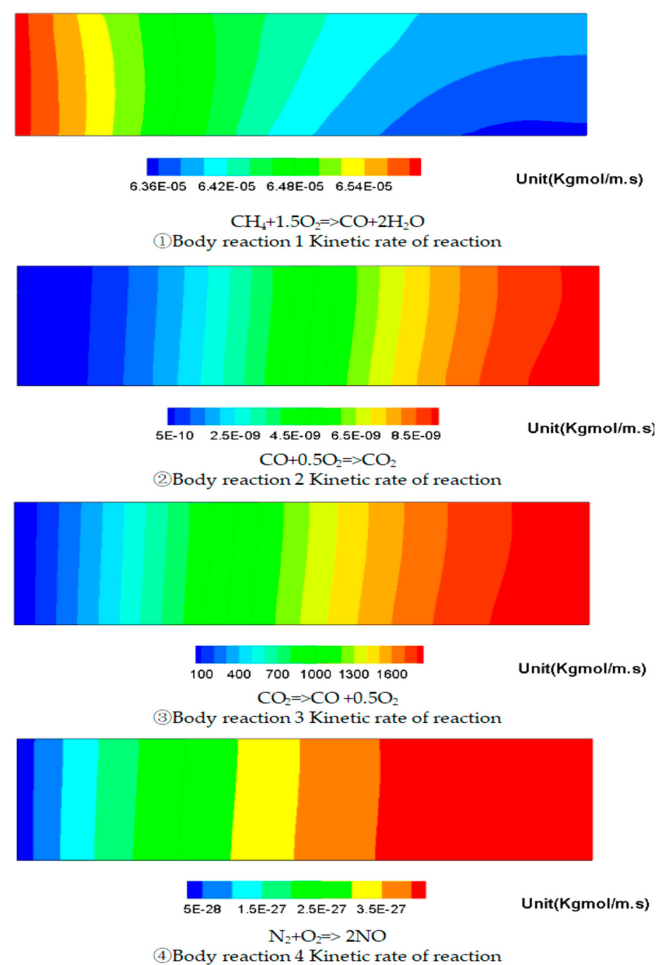
tion distribution map, respectively. The distribution of H<sub>2</sub>O and CO<sub>2</sub> increases with the depth of the hole and is evenly distributed on the same hole depth section.



**Figure 5.** Distribution of product mass fraction: (a) H<sub>2</sub>O mass fraction distribution; (b) CO<sub>2</sub> mass fraction distribution.

### 3.1.3. Kinetic Rate of Reaction

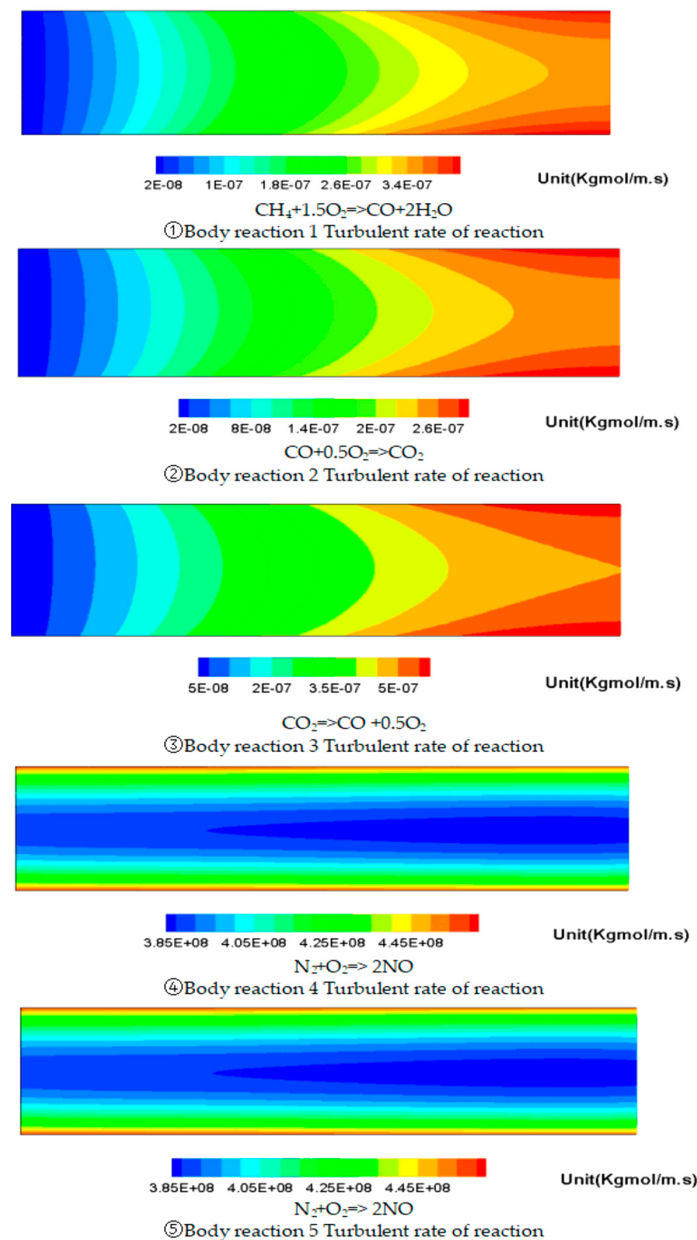
According to the body reaction mechanism shown in Table 1 [29], the body-reaction dynamic reaction velocity distribution diagram includes the following four diagrams (there is no Reaction 5; Reaction 5 is the same as Reaction 4, and the software is classified as one). As shown in Figure 6, except for the dynamic reaction velocity of Body Reaction 1 in which the inlet is larger than the interior and gradually decreases along the hole depth direction, the dynamic reaction velocity of the other three individual reactions is such that the inlet is smaller than the interior and gradually accelerates along the hole depth direction.



**Figure 6.** Kinetic rate of the reaction distribution diagram.

### 3.1.4. Turbulent Rate of Reaction

According to the reaction mechanism shown in Table 1, the turbulent reaction velocity distribution map includes the following five diagrams. As shown in Figure 7, the turbulent reaction velocity of Volume Reactions 1–3 is that the inlet is smaller than the inside and gradually accelerates along the depth of the hole. Then, as the hole depth increases, the reaction speed on the same section of the inner wall of the channel becomes more uneven, and the wall surface becomes larger than the center. The turbulent reaction velocity of Body Reactions 4 and 5 is evenly distributed as a whole and does not change significantly with the hole depth. Furthermore, the overall distribution is axisymmetric along the center line of the hole, and the wall surface is larger than the center.

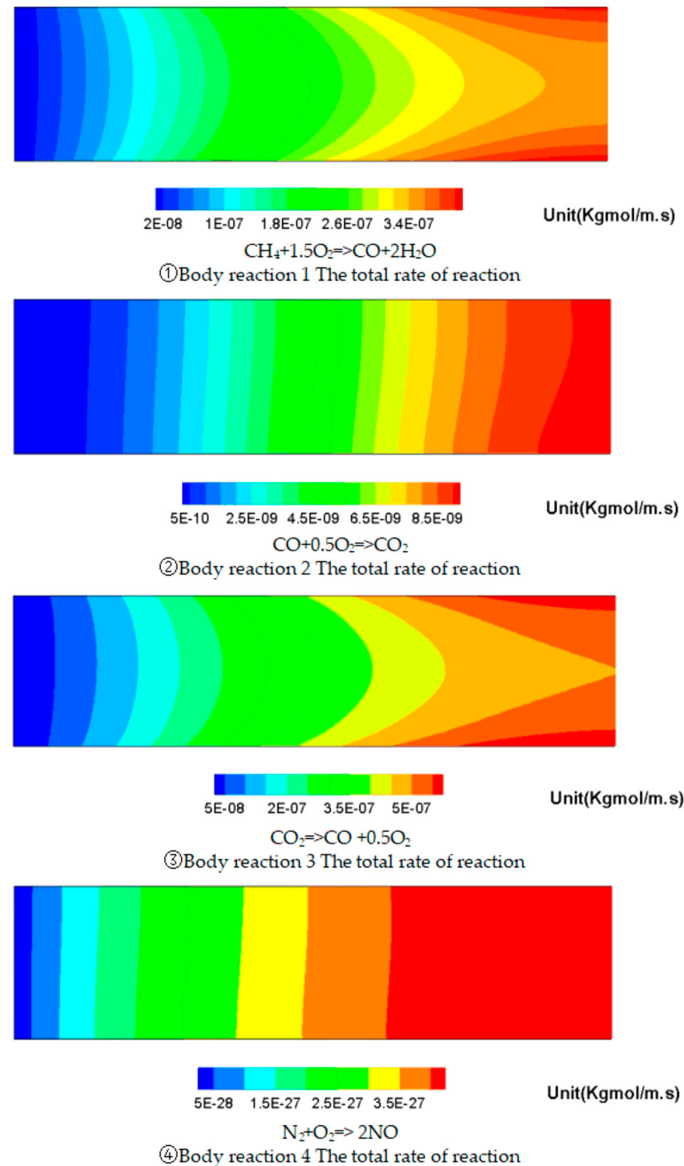


**Figure 7.** Turbulent rate of the reaction distribution diagram.

### 3.1.5. Total Reaction Rate

The total reaction speed is shown in Figure 8. The overall reaction speed is gradually accelerated along the hole depth direction, among which Body Reactions 2 and 4 exhibit linear acceleration along the hole depth direction, and the reaction speed is more uniform

in the same section. Meanwhile, Body Reactions 1 and 3 exhibit acceleration along the hole depth direction simultaneously, and the reaction speed on the same hole depth section indicates that the side wall is larger than the center.



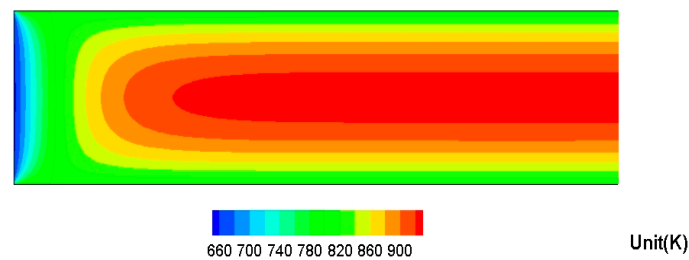
**Figure 8.** Total rate of the reaction distribution diagram.

### 3.2. Analysis of the Microporous Surface Reaction Combustion Simulation

The surface reaction of micropores occurs on the inner wall of the channel, which is affected by the supported catalyst and coexists with the bulk reaction.

#### 3.2.1. Surface Reaction Temperature Field

Figure 9 shows the temperature field of the combustion reaction on the inner wall surface of the micropore after loading the platinum/palladium catalyst. Unlike the bulk reaction, due to the reaction of the wall, the temperature of the whole region is higher, and the temperature inside the hole is considerably higher than that of the orifice. The simulation reveals that the temperature difference is up to  $300^\circ\text{C}$ . Near the orifice, the temperature on the section at the same hole depth is evenly distributed. Additionally, along the hole depth direction, the center temperature is higher than the side wall temperature as a whole and presents a circular distribution.

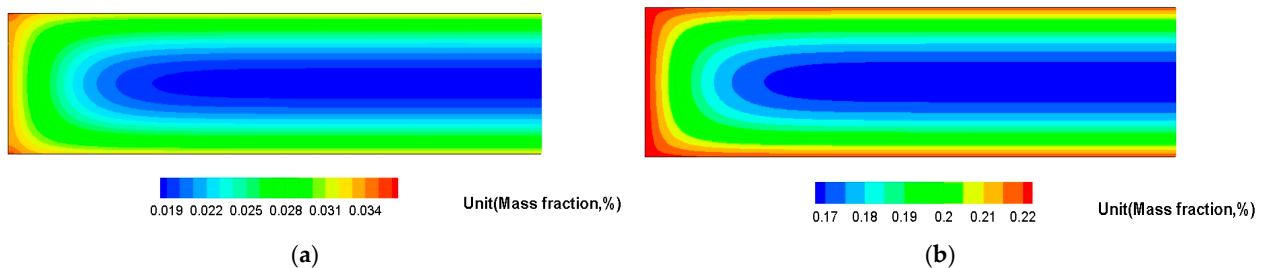


**Figure 9.** Surface reaction temperature field distribution.

### 3.2.2. Species Mass Fraction

#### (1) Distribution of the reactant mass fraction

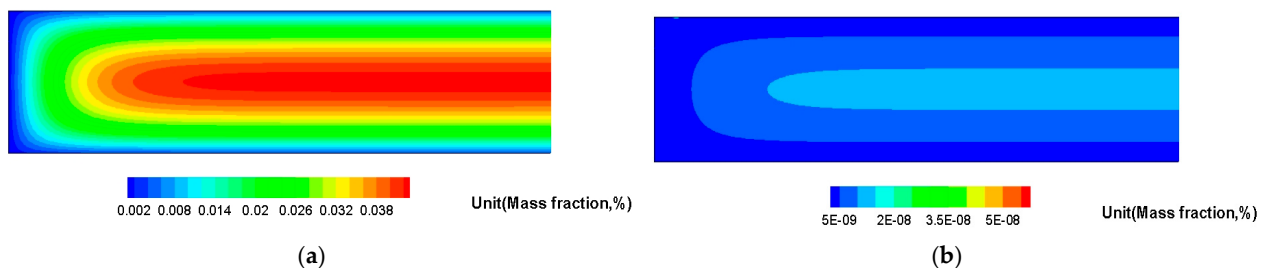
Figure 10a shows the distribution of methane mass fraction. The concentration is high at the entrance. However, after the reaction, the concentration gradually decreases along the depth of the hole. Upon exceeding a certain depth of the hole, methane shows a symmetrical distribution along the center line of the hole as the axis and the side wall become larger than the center. Meanwhile, Figure 10b shows the distribution of oxygen mass fraction, which is similar to that of methane. The difference is that the overall concentration near the inlet is higher than that of methane, and the overall distribution is annular.



**Figure 10.** Distribution of the reactant mass fraction: (a) methane mass fraction distribution; (b) oxygen mass fraction distribution.

#### (2) Distribution of the product mass fraction

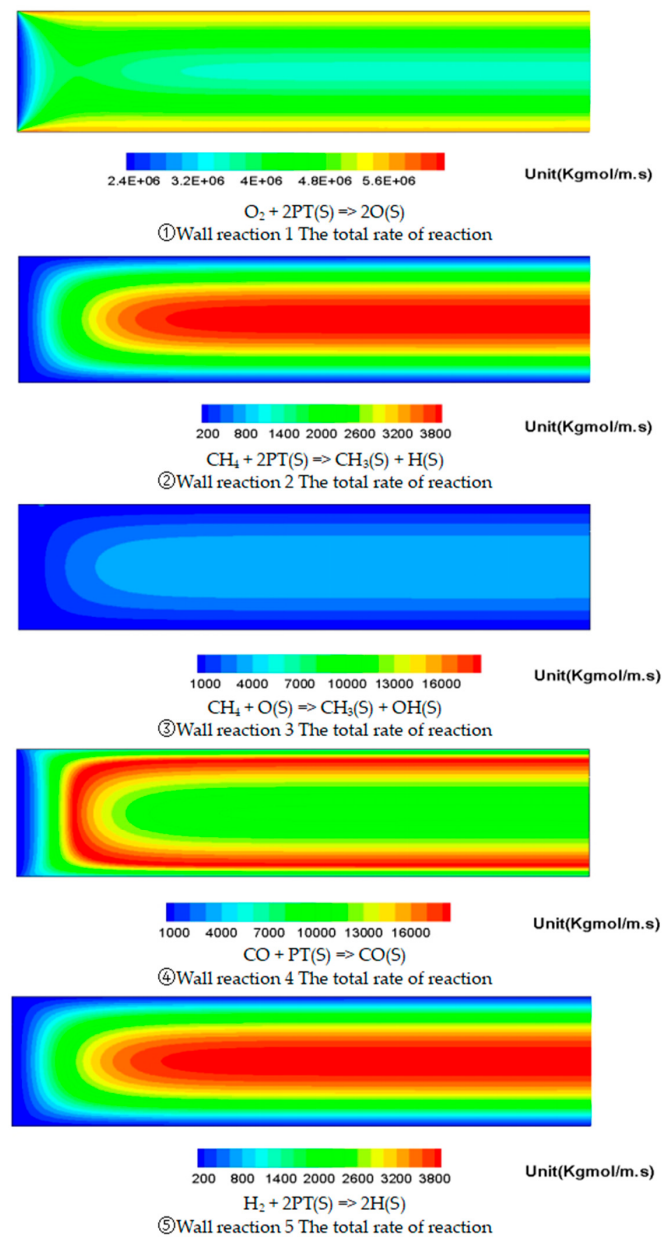
After the reaction, the obtained products are mainly  $H_2O$  and  $CO_2$ , as shown in Figure 11. Particularly, Figure 11a,b show the  $H_2O$  concentration distribution map and the  $CO_2$  concentration distribution map, respectively. The distribution becomes larger with increasing hole depth, which is opposite to the phenomenon shown by the mass fraction distribution of the reactants. The accuracy of the reaction formula is verified reversely. The products are evenly distributed on the cross section of the same hole depth. Based on the reaction equation involved in the wall reaction mechanism [30], more than its own volume of  $H_2O$  will be produced while generating  $CO_2$ . Therefore, the mass fraction distribution of  $H_2O$  in the overall distribution of the products is much higher than that of  $CO_2$ .



**Figure 11.** Distribution of the product mass fraction: (a)  $H_2O$  mass fraction distribution; (b)  $CO_2$  mass fraction distribution.

### 3.2.3. Total Reaction Rate

The total reaction rate is shown in Figure 12. Overall, it gradually accelerates along the hole depth direction, and reaches stability after exceeding a certain hole depth. It is also symmetrically distributed along the center line of the hole. When Reaction 1 exceeds a certain hole depth, the reaction speed on the same section shows that the side wall is larger than the center; after the Reactions 2, 3, and 5 exceed a certain hole depth, the reaction speed on the same section shows that the center is greater than the side wall. Meanwhile, Reaction 4 is different from other reactions; it first accelerates and then decreases along the depth of the hole. After exceeding a certain hole depth, it first increases and then decreases from the side wall to the center line, although the reaction speed is also symmetrically distributed along the center line of the hole.



**Figure 12.** Total reaction rate distribution diagram.

### 3.3. Analysis of the Impact of Process Parameters on Combustion Reaction

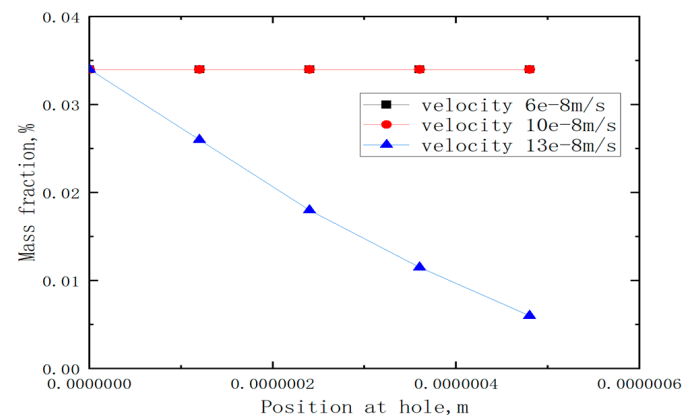
The process parameters of the sensor-sensitive element have an important influence on the micropore combustion reaction of methane [32]. The results showed that the position of

the microhotplate installation is different, and the response output tends to change greatly. The simulation analyses of the three influencing factors of the inlet velocity of the microhole, inlet methane concentration, and the size of the microhole itself caused by the influence of the process parameters provide theoretical support for the subsequent sensor design.

### 3.3.1. Influence of Process Parameters on Bulk Reaction

#### (1) Inlet velocity

As shown in the Figure 13 and Table 4, with increasing inlet velocity, the methane consumption (combustion) ratio increases. The images of inlet velocities,  $6 \times 10^{-8}$  m/s and  $1 \times 10^{-7}$  m/s, coincide, indicating that when the flow rate is between them, it will not affect the methane-burning rate. When the flow rate exceeds  $1 \times 10^{-7}$  m/s, the change in methane consumption and the burning rate become particularly obvious.



**Figure 13.** Effect of inlet velocity on combustion reaction.

**Table 4.** Effect of inlet velocity on combustion reaction.

| Inlet Velocity      | Inlet Methane Mass Fraction | Outlet Methane Mass Fraction | Combustion Ratio (%) |
|---------------------|-----------------------------|------------------------------|----------------------|
| $6 \times 10^{-8}$  | 0.034                       | 0.03391                      | 0.27                 |
| $1 \times 10^{-7}$  | 0.034                       | 0.033997                     | 0.0088               |
| $13 \times 10^{-8}$ | 0.034                       | 0.0055258                    | 83.7                 |

#### (2) Inlet concentration

As shown in the Figure 14 and Table 5, the methane combustion ratio increases with the increasing inlet methane mass fraction. Furthermore, the combustion ratio and concentration are changed in multiples so that it can be inferred that they are linear. Notably, the burning rate of methane is constant at different concentrations; hence, the change in methane concentration in the bulk reaction does not cause a change in the burning rate.

#### (3) Pore size

As shown in the Figure 15 and Table 6, it can be seen that the methane combustion ratio changes linearly with the pore size. With the increasing pore size, the methane combustion ratio first increases and then decreases. Taking the pore depth of 0.00000024 m as the node, before that, the methane burning rate of different pore sizes fluctuates greatly; however, there is no violent fluctuation in the latter. Additionally, the smaller pore size at 60 nm has the largest change in the burning rate. When the pore size is 150 nm, the change is the most stable, and the overall value is also higher than the other two pore sizes. A finer delineation and testing of the aperture size has been made compared to the overall size of 300 nm in previous studies [5].

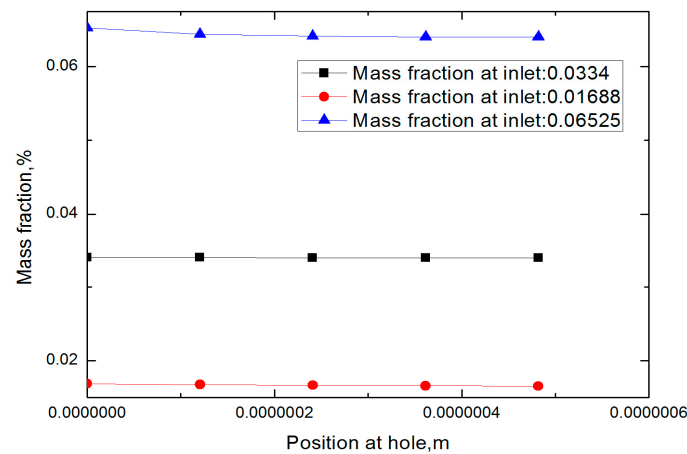


Figure 14. Effect of inlet methane concentration on combustion reaction.

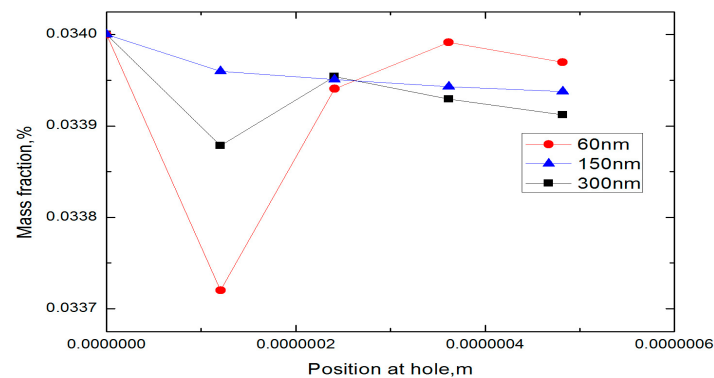


Figure 15. Effect of pore size on combustion reaction.

Table 5. Effect of inlet methane concentration on combustion reaction.

| Inlet Concentration   | Inlet Methane Mass Fraction  | Outlet Methane Mass Fraction | Combustion Ratio (%) |
|-----------------------|------------------------------|------------------------------|----------------------|
| $1.69 \times 10^{-2}$ | $1.687500067 \times 10^{-2}$ | $1.653965376 \times 10^{-2}$ | 1.99                 |
| $3.40 \times 10^{-2}$ | $3.400000185 \times 10^{-2}$ | $3.391203284 \times 10^{-2}$ | 0.26                 |
| $6.53 \times 10^{-2}$ | $6.525000185 \times 10^{-2}$ | $6.399093568 \times 10^{-2}$ | 1.93                 |

Table 6. Effect of pore size on combustion reaction.

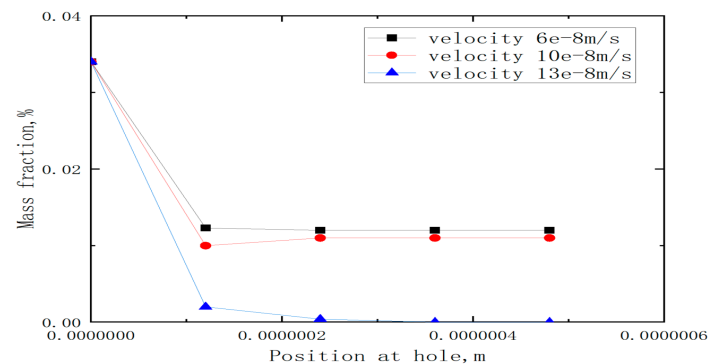
| Pore Size | Inlet Methane Mass Fraction  | Outlet Methane Mass Fraction | Combustion Ratio (%) |
|-----------|------------------------------|------------------------------|----------------------|
| 60 nm     | $3.400000185 \times 10^{-2}$ | 0.03391203284                | 0.26                 |
| 150 nm    | $3.400000185 \times 10^{-2}$ | 0.03393090516                | 0.20                 |
| 300 nm    | $3.400000185 \times 10^{-2}$ | 0.03390500322                | 0.28                 |

### 3.3.2. Effect of Process Parameters on Surface Reaction

#### (1) Inlet velocity

As shown in the Figure 16 and Table 7, compared to the no-wall reaction, in the interior of the wall, the adsorption amount of methane is increased due to the participation of the catalyst, and the speed of methane passing through the channel is accelerated, thereby greatly increasing the combustion ratio and burning rate of methane. As the inlet velocity increases, the combustion ratio increases rapidly. When the inlet velocity is between  $6 \times 10^{-8}$  and  $1 \times 10^{-7}$  m/s, the methane consumption increases slowly; in comparison,

when the inlet velocity exceeds  $1 \times 10^{-7}$  m/s, the methane consumption increases rapidly. Overall, compared to the bulk reaction, the methane consumption and burning rate changed significantly at different inlet velocities.



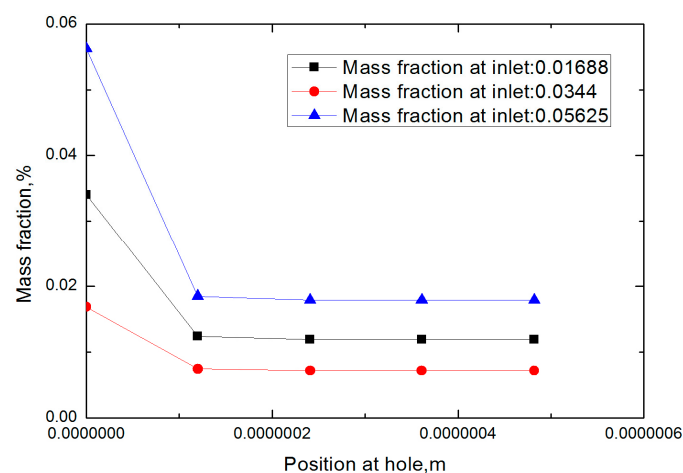
**Figure 16.** Effect of inlet velocity on combustion reaction.

**Table 7.** Effect of inlet velocity on combustion reaction.

| Inlet Velocity      | Inlet Methane Mass Fraction | Outlet Methane Mass Fraction | Combustion Ratio, % |
|---------------------|-----------------------------|------------------------------|---------------------|
| $6 \times 10^{-8}$  | 0.03400000185               | 0.01191107742                | 65.0                |
| $1 \times 10^{-7}$  | 0.03400000185               | 0.01071531605                | 68.5                |
| $13 \times 10^{-8}$ | 0.03400000185               | 0.00000363869                | 100                 |

## (2) Inlet concentration

As shown in the Figure 17 and Table 8, similar to the bulk reaction, the combustion ratio increases with the increasing inlet concentration. The difference is that the methane consumption and burning rate change considerably from the orifice position to the depth of 0.00000012 m. When the hole depth reaches a certain depth, the burning rate does not change considerably. However, methane consumption still increases with increasing inlet concentration. Hence, the reaction interval was clarified compared to the previous conclusion that the reaction was only within the hole [31].



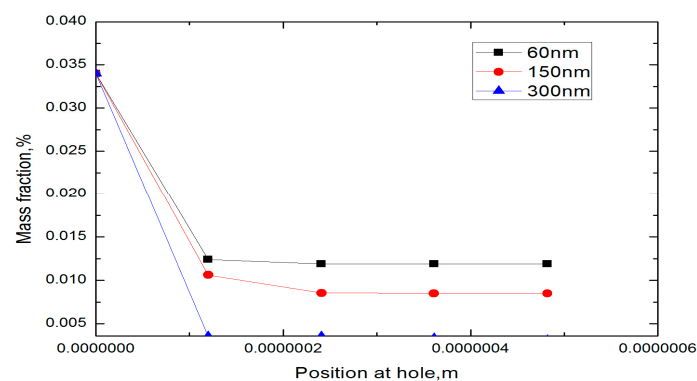
**Figure 17.** Effect of inlet methane concentration on combustion reaction.

**Table 8.** Effect of inlet methane concentration on combustion reaction.

| Inlet Concentration | Inlet Methane Mass Fraction | Outlet Methane Mass Fraction | Combustion Ratio, (%) |
|---------------------|-----------------------------|------------------------------|-----------------------|
| 0.01687500067       | 0.01687500067               | 0.00717461854                | 57.5                  |
| 0.03400000185       | 0.03400000185               | 0.01191107742                | 65.0                  |
| 0.05624999851       | 0.05624999851               | 0.01790973172                | 68.2                  |

## (3) Pore size

As shown in the Figure 18 and Table 9, unlike the bulk reaction, the combustion ratio increases with increasing pore size. When the pore size exceeds 150 nm, the rate change is particularly obvious, and the combustion ratio is close to 100%. Changes in methane consumption and the burning rate are greatly improved from the orifice position to the depth of 0.00000012 m. From this position to the outlet of the orifice, the burning rate of the 150 nm aperture has a slight downward trend, and the burning rate of the other two apertures has no obvious change; however, methane consumption continues to increase with increasing aperture. While analyzing with body-reaction, the aperture size at the wall should be controlled so that it is larger than 300 nm, and the aperture should be transitioned from 150 nm to the inside. In doing so, the gradual structure of the aperture is realized. Thus, the 300-nm aperture size of previous studies can be improved, and the performance of this type of methane sensor in coal mine underground can be enhanced.

**Figure 18.** Effect of pore size on combustion reaction.**Table 9.** Effect of pore size on combustion reaction.

| Pore Size | Inlet Methane Mass Fraction   | Outlet Methane Mass Fraction | Combustion Ratio, % |
|-----------|-------------------------------|------------------------------|---------------------|
| 60 nm     | $3.400000185 \times 10^{-22}$ | 0.0129                       | 62.1                |
| 150 nm    | $3.400000185 \times 10^{-2}$  | 0.0085                       | 75.0                |
| 300 nm    | $3.400000185 \times 10^{-2}$  | 0.0031                       | 90.9                |

#### 4. Conclusions

In this study, a 3D model of a sensor was established, and the changes observed with respect to the reaction temperature field, reaction rate, and process parameters of methane combustion inside the micropore were simulated and analyzed. The results show that the mass fraction of reactants tended to decrease from the orifice to the interior; meanwhile, the products and the total reaction rate gradually increased. Furthermore, the surface reactions were distributed in a circular pattern along the wall and were symmetrical with the center line of the pore. Except for the reactants, each substance or variable increased from the side wall to the center, which was more regular than that observed in the bulk reaction. Additionally, the methane consumption and combustion rate changed

considerably from the orifice to a 0.00000012 m hole depth, after which the combustion rate did not exhibit a significant change. Thus, the best combustion position of methane inside the orifice is determined to be at depths of 0–0.00000012 m, which complements previous conclusions regarding the reaction inside the orifice. Furthermore, the methane combustion rate increases with the increasing inlet concentration and velocity, proportional to the concentration change. When the inlet flow rate is below  $1 \times 10^{-7}$  m/s, the combustion rate increase is not obvious; however, when the inlet flow rate exceeds  $1 \times 10^{-7}$  m/s, the methane combustion rate changes considerably faster. These findings are more accurate compared with the uniform velocity concept used in previous studies. The pore size at the inlet should be controlled at 150 nm, and the optimal pore size at the wall should be larger than 300 nm and should not be too high. Otherwise, it will lead to too much internal space and lower temperature, resulting in a lower methane consumption rate. The pore size was measured more finely compared to 300 nm in previous studies. The results of this study are important for the adjustment and control of porosity and pore meshes in future simulations and experiments. The pore size length can be shortened, and the effective reaction interval can be increased in future studies.

**Author Contributions:** Conceptualization, B.S.; methodology, T.Z.; software, T.Z.; validation, W.L., T.Z. and X.Q.; formal analysis, W.L. and T.Z.; investigation, X.L.; data curation, X.L.; writing—original draft preparation, B.S. and T.Z.; writing—review and editing, B.S.; supervision, X.Q. All authors have read and agreed to the published version of the manuscript.

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