Effects of products from heterogeneous reactions on homogeneous combustion for H₂/O₂ mixture in the micro combustor

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Abstract

Three-dimensional computational fluid dynamics (CFD) models with detailed homogeneous (gas phase) and heterogeneous (catalytic) chemistries were performed inside a rectangular micro-combustor. The simulation model, based on the chemical reaction kinetics, was validated by experimental data. The effects of the intermediate and final product from heterogeneous reactions on the homogeneous combustion in a catalytic combustor were discussed. The results of numerical simulation show that the presence of intermediate can promote the fuel conversion ratio. The addition of final product can significantly decrease the flame temperature and fuel conversion ratio attributed to the heat loss of reaction and weakness in the combustion intensity. Similar results are obtained when all the products are added as compared to only the addition of the final product. Suppression effect of the final product on homogeneous combustion displays a dominant role among the effects of all products. The combustor performance can be commonly promoted in the hetero-/homogeneous combustion system due to the existence of catalysis.

Keywords: Heterogeneous and homogeneous combustion; desorption; catalysis; micro combustor

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1. Introduction

Nowadays, with growing interest in developing portable power generation systems, the attention towards combustion in meso and micro scale channels is significantly enhanced [1, 2]. Combustion in the channels with fossil fuels as a power source has many advantages due to their high energy density, availability, easy storage and low cost. However, there are also some obstacles in the development of meso/micro scale reactors, such as low combustion efficiency and instability of flame [3-5]. Furthermore, with the decrease of the size of meso/micro scale reactors thereby increasing the surface-to-volume ratio, the defect of the reactors is more obvious, except for micro thermophotovoltaic (MTPV) system and catalytic combustors [6-9]. In this regard, catalytic reactions can extend the classical flammability limits and improve combustion stability even in the presence of high heat losses [1, 2, 10]. It is confirmed by Fanaee and Esfahani [11, 12] that the presence of a catalytic wall can decrease the quenching distance to extend the flammability limits in meso/micro scale reactors as compared to the non-catalytic wall case.

The interactions between the heterogeneous and homogeneous reactions are very complex and have received increasing attention, but it is still not clear. It has been demonstrated that these interactions include the promotion of homogeneous reactions due to catalytically induced exothermicity and the inhibition of heterogeneous reactions on the homogeneous reactions mainly caused by competition of fuels and oxidizers of the heterogeneous reactions versus homogeneous reactions [13]. Pizza et al. [14, 15] demonstrated the potential of catalytically-coated walls in mitigating intrinsic flame instabilities of meso/micro scale channels. Wang et al. [16] compared the reaction intensity between catalytic and non-catalytic combustors. The results showed that the catalytic combustor displayed a high stability and weak reaction intensity. In addition, the catalytic combustion

effectively improved the homogenous combustion efficiency in a micro-reactor [17]. Zade et al. [18] also numerically investigated the importance of gas-phase and surface reactions for H_2 /air mixture in the planar micro-channel, indicating that the lean limitations of gas-phase reactions became negligible when compared to the surface reactions [19]. Chen et al. [20] clarified and highlighted the effects of heterogeneous reaction for H_2 /air mixture by numerical simulation. The overall picture of gas-phase and surface reaction interactions was depicted, under inlet velocity versus a function of channel diameter. Three regions were divided in the picture and separately dominated by different reactions. Veeraragavan et al. [21-23] investigated the flame stability and stabilizing mechanism using thermally orthotropic walls in the micro combustors, and this achievement can be used for guiding the effect of exothermicity induced by catalytic reaction.

In the heterogeneous reaction, the reactants are adsorbed on catalytic surface to participate in the reaction, and the products desorb and diffuse outwards eventually to the bulk gas after reaction [24]. Smyth et al. [25, 26] investigated experimentally, the preheated methane/air and propane/air mixtures over platinum (Pt) foil leading to the heterogeneous reactions, which was sustained on the surface. The results showed that the leading edge zone of the flat plates of combustion was established and could be used for burner miniaturization. Subsequently, Badra et al. [27] addressed the interactions between homogeneous and heterogeneous reactions for different hydrocarbons over Pt foil at different inlet temperature (T_{jet}), equivalence ratio (ϕ), and Reynolds number (Re) and simulated the catalytic combustion using FLUENT. The results showed that the gas and surface chemistries affected a few species such as CO, CO₂, H₂, and H₂O depending on the conditions of the co-flowing mixture, and minor species such as CH₃, CH₂O, O, HCO, and OH were largely controlled by gas-phase chemistry. However, in the coupled hetero-/homogeneous chemistries combustor, Vlachos [28] considered that the

homogeneous ignition was inhibited by catalytic formation of H_2O and could be affected by multi-component transport phenomena. Comparison of simulation results and experimental data, showed that the adsorption of hydrogen atoms to the surface inhibited homogeneous ignition in a stagnation-point flow reactor. For the competition between the homogeneous and heterogeneous reactions near the catalytic surface, Deutschmann et al. [29] proved that the competition was mainly driven by sticking probability of species on the surface.

It is evident from these studies that in the coupled hetero-/homogeneous reactions, the interactions between the homogeneous and heterogeneous reactions are still not fully understood under numerous controlling parameters, especially for desorbed products effect. In this work, numerical simulations were carried out by detailed gas-phase and surface reaction mechanisms for H_2/O_2 mixture over platinum catalyst. The purely heterogeneous reaction mode was employed to obtain the gaseous species at the exit in the first model, including the intermediate, final product and residual reactants. Then the various combinations of products were taken as the boundary conditions of the inlet in the second model. In this way, this paper presents a comprehensive and systematic study on the effects relating to the desorbed gaseous species from heterogeneous reactions, namely the effects of intermediate, final product and all desorbed gaseous species on the homogeneous combustion.

2. Physical and Mathematical Description

2.1. Physical Model

Two three-dimensional simulation models are performed to simulate the reactive gas flow and reaction characteristics, using the commercial CFD code FLUENT [30]. For the first model (see Fig. 1, model 1), it is a rectangular channel, with 1 mm length (- x , L), 10 mm width (- y , W), 1 mm height (- z , H), and 0.4 mm wall thickness (W_s). In the CFD modeling, the platinum catalyst with 1mm length is

coated on the inner surface of the silicon carbide (SiC) wall with a density of $2.72 \times 10^{-9} \text{ mol/cm}^2$. The configuration of the next simulation model (see Fig. 1, model 2) is similar to model 1, but with a 10 mm length (-x, L_2). During the operation process, premixed hydrogen/oxygen mixture flow into the straight parallel channel through a rectangular inlet which is located at the left of the combustor, and the burned gas will be expelled out from an outlet at the other end of the combustor. In the second computation model, an optimized grid with 140400 cells is employed as shown in Fig. 2. The refined grids are utilized in the reaction region near the wall for obtaining high-resolution boundary data and analyzing surface layer catalysis chemistry in the computational domain.

Fig. 1. Schematic of the computational domain: Model 1 is 1 mm in length and the inner wall is coated with platinum catalyst. Model 2 is 10 mm in length, and the catalyst segment is 1 mm length at the inlet in the inner surface.

Fig. 2. Centerline temperature profiles of combustor at a inlet flow rate of 26.4064 g/h with different mesh densities

2.2. Methods of model building

In this simulation, the inlet Reynolds number is less than or equal to 88 (based on the maximum flow rate of 26.4064 g/h) via the calculation, so the laminar model is adopted [31]. The flow can be reasonably considered as continuum (the Knudsen number is less than the critical value of 0.001). The main governing equations are discretized by a first-order upwind scheme in the numerical model, including steady-state Navier–Stokes equations, mass and energy conservation equations, and species conservation equations, respectively [30]. A piecewise polynomial fitting method is employed to calculate the specific heat of the species. The density and specific heat of the hydrogen-oxygen mixture are calculated by incompressible ideal gas law and mixing law, respectively. The mixture gas thermal conductivity and viscosity are calculated as a mass fraction weighted average of all species, and the kinetic-theory is selected for mass diffusivity calculation of mixture. SIMPLE algorithm is chosen to deal with the pressure-velocity coupling. The simulation convergence is declared when the residuals of all governing equations approach steady states. With the convergent criteria, the results reported in this work have been achieved with residuals smaller than 10^{-6} .

The boundary conditions are set as follows. The mass-flow-inlet and outflow boundary conditions are specified at the inlet and outlet, respectively. A uniform velocity profile is adopted at the inlet, and the hydrogen-oxygen equivalence ratio is 1.0. In our study, the atmospheric pressure (101 KPa) and temperature (300 K) are specified. Therefore, the temperature of inlet mixture and the initial temperature for the chamber solid walls are fixed at 300 K. A non-slip boundary condition is imposed on each wall. The effects of surface to surface radiation between the inner surfaces of the combustor

are considered using the discrete ordinates (DO) model [31]. The heat loss from the exterior wall to the ambient air is calculated via Eq (1). The mixed thermal conditions are set for outer wall, and the convective heat transfer coefficient and wall emissivity are considered [32].

$$q'' = h(T_w - 300) + \varepsilon \sigma (T_w^4 - 300^4) \quad (1)$$

where T_w is outer surface temperature, h is natural convection coefficient considered constant value, 20 W/m²/K, $\sigma = 5.67 \times 10^{-8}$ W/m²/K⁴ is Stephan-Boltzmann constant and ε is the solid surface emissivity (0.77 in this study).

A skeletal gas phase reaction mechanism proposed by Miller and Bowman for hydrogen-oxygen mixture is used in the computation model, which has 9 species and 19 reversible elementary reactions [33]. The surface chemistry mechanism for hydrogen over platinum is taken from Deutschmann et al [29]. This simulation includes five surface species: Pt(s), H(s), H₂O(s), OH(s) and O(s).

2.3. Validation of the Model

In order to validate the numerical model and chemical mechanisms used in this study, the experimental validation has been conducted on the micro planar reactor with hydrogen-oxygen mixture, and the experimental results are compared with the simulation data under the same conditions. The experimental setup is given in our previous study [32], the temperature distribution on the external surface of the combustor is measured by an infrared thermal imager (Camera model: Thermovision TM A40) and recorded by a computer. In that apparatus, the maximum measurable temperature is 2000°C and measuring accuracy is $\pm 2\%$. Fig. 3 shows the centerline temperature profiles on the external surface both by experiment and simulation with non-/catalytic wall (1mm length). Comparing simulation and experimental results, the maximum deviation between simulation and experimental results is 1.1% (with non-catalytic wall) and 2.3% (with catalytic wall) respectively, confirming a

reasonable accuracy of the numerical model adopted in this work.

Fig. 3. Comparison of centerline temperature profiles on the external surface both by experiment and simulation with non-/ catalytic wall.

3. Results and discussion

3.1. Combustion characteristics of heterogeneous reaction

In this work, the purely heterogeneous reaction model was carried out by numerical simulation under adiabatic condition. The initial conditions at inlet for the reactants are set as follows: mass flow rate of 26.4064 g/h, incoming mixture temperature of 300K and equivalent ratio of 1.0. Fig. 4 shows the contours of the OH and H₂O concentration distributions in the micro catalytic reactor. The simulation results show that the characteristic of heterogeneous combustion is very significant, accompanying with the occurrence of reactions on the wall and a lower reaction temperature. It is worth noting that the hydrogen conversion ratio in this reactor is only 0.26. In this simulation, the gaseous products are desorbed from catalytic wall via desorption reactions which are included in the detailed surface chemistry mechanism [24, 29]. Then the mean amount of gaseous species (various products and residual reactants) at the outlet are gained by numerical simulation in the first model, as

shown in Table 1.

Fig. 4. Computed contours of OH concentration distributions (left column) and H₂O concentration distributions (right column) in the micro catalytic reactor.

Table 1 Mass fraction of gaseous species at the outlet gained by numerical simulation in the first model

Gaseous species	Value (mass fraction)
H ₂	0.073606
O ₂	0.594239
H ₂ O	0.33215162
OH	0.00000338

3.2. Effects of gaseous species

In order to understand the effect of the heterogeneous reaction products on homogeneous combustion, the effects of products addition on homogeneous combustion for the residual reactant were investigated. Two reaction modes were performed in the second model, including the homogeneous reaction mode, and coupled heterogeneous and homogeneous reaction mode. In this work, the above two modes both have the stoichiometric ratio and inlet flow rate of 26.4064 g/h, which are marked Case A and B, served as the reference cases, respectively. The various combinations of products are added in the residual reactant, and the ultimate combinations were taken as the boundary conditions of the inlet in the second model, as shown in Table 2. This is aimed at grasping the effects of heterogeneous reactions on the homogeneous combustion.

Table 2 Inlet boundary conditions from different cases in the homogeneous reaction mode

Case	Inlet gas velocity (g/h)	Specified species
C	17.6353	H ₂ , O ₂
D	26.4062	H ₂ , O ₂ , H ₂ O
E	17.6355	H ₂ , O ₂ , OH
F	26.4064	H ₂ , O ₂ , OH, H ₂ O

3.2.1. Effects of intermediate

In the combustion reactions of hydrogen, the effects of intermediates on homogeneous combustion are always to be mentioned. Therefore, the desorbed intermediate from heterogeneous reactions (OH) is employed to indicate an obvious impact on the homogeneous combustion in the coupled reactions, that is the Case E. The Case B and Case C serve as the reference cases.

Fig. 5 shows the computed contours of the temperature and OH concentration distributions in the micro-reactor for all cases. It can be seen from the temperature distributions, the high temperature region in all cases displays a cone shape. However, for the maximum temperature level, Case B is only 2530 K, other cases are about 2650 K. Furthermore, by comparison of the cases except Case B, it is indicated that the computed contours of temperature and OH concentration in the channel have a similar distribution. As known, the OH concentration distributions commonly denote the reaction zone and high temperature zone in the homogenous combustion [13, 20]. Therefore, in the Case C and E, the maximum OH concentration level and the size of the higher concentration zone are roughly similar, which indicates that the intermediate has no apparent effect on the homogenous combustion for the temperature and OH concentration distributions. There exists the same tendency for the temperature and OH concentration in the centerline of the channel for the later two cases. For the Case B, the adsorbed species are depleted near the catalytic surface, depending on the surface coverage of sites. In addition, the contour plot displays a low OH concentration region near the catalytic wall, revealing that the heterogeneous reactions have the inhibition effect on the homogeneous combustion caused by the

competition of intermediate between heterogeneous reaction and homogeneous reaction [24, 29]. The desorbed intermediate can promote the homogeneous combustion, but the promotion is weak due to a small amount of the desorbed intermediate. Compared with the OH concentration distributions between the Case B and C, a low OH concentration region near the catalytic wall can indicate that the absorption effect of intermediate is greater than that of the desorption.

Fig. 5. Computed contours of temperature (left column) and OH concentration distributions (right column) in the micro-reactor for Case B, C and E .

However, it can be observed that the fuel conversion ratio and the mean outlet temperature are different respectively, as shown in Table 3. For the Case B, the fuel conversion ratio is only 0.987 which is lower than that of other cases, but the mean outlet temperature (1603.1 K) is higher than that of other cases. In the Case E, it shows an increase in the fuel conversion ratio and a decrease in the temperature when compared with the Case C, indicating that the addition of intermediate can promote the fuel combustion efficiency and decrease the exhaust temperature [24]. In other words, the desorption of intermediate from the heterogeneous reactions improve homogeneous combustion. However, the fuel conversion ratio of Case E is 0.001 higher than that of Case C due to the lower

amount of the desorbed intermediate. It is further concluded that the promotion of desorbed intermediate on homogeneous combustion is weak.

Table 3 Fuel conversion ratio and mean outlet temperature for different cases.

Case	Mean outlet temperature (K)	Fuel conversion ratio
B	1603.1	0.987
C	1425.1	0.994
E	1423.7	0.995

3.2.2. Effects of final product

It is demonstrated that the intermediate can promote the homogeneous combustion efficiency, and the final product also plays an important role in combustion. Therefore, the Case D should be investigated, and the Case B and Case C serve as the reference cases.

The temperature and OH concentration profiles on the centerline of the channel are shown in Fig. 6a and Fig. 6b, respectively. It can be seen from Fig. 6a that the temperature first increases and then slowly decreases. By comparing the three cases, the maximum temperature (2650.5 K) of Case C is higher than that of the other cases, and the peak temperature (only 2292 K) of Case D is the lowest. It can be found that for the Case D, the peak temperature is significantly lower due to the addition of final product, resulting in a heat loss from the reactions. Meanwhile, the combustion reaction is a reversible reaction, the existence of products can hinder the forward reaction and decrease forward reaction rate, ultimately leading to a decrease in reaction intensity. As shown in Fig. 6b, the OH concentration shows a sudden increase first and then decrease, indicating that the reaction intensity of Case D decreases. In Case D, the peak of OH concentration is about half that of Case C. The homogeneous reaction intensity of Case D is lower than that of Case C.

This result demonstrates that the addition of final product (H_2O) can significantly decrease the gaseous temperature in reaction zone and make the premixed flame easier to extinguish. Moreover, for

the chemical influence of adding water, the high third-body efficiency arises in the homogeneous reaction $\text{H} + \text{O}_2 + \text{M} = \text{HO}_2 + \text{M}$, where M represents any third body, resulting in the chain-breaking of the reaction. The water retards the homogeneous combustion, among others, it assists efficiency in three body reactions. While the concentration of the third body is enhanced, the final product inhibition is more obvious due to the existence of many other reactions in the presence of M [34]. Thus, it can be concluded that the desorption of final product can suppress the homogeneous combustion effectively.

Fig. 6. Temperature (a) and OH concentration (b) profiles on the centerline of channel

3.2.3. Effects of all products

In the heterogeneous and homogeneous coupled reactions, the intermediate and final product are simultaneously desorbed from the heterogeneous reactions and then can affect the homogeneous combustion. Therefore, the effects of all gaseous species on the homogeneous combustion should be investigated in the coupled reactions as the Case F. Also, other cases are regarded as the reference cases, including Case A and Case B.

Fig. 7 shows the computed contours of the temperature and OH concentration distributions in the micro-reactor for all cases. As can be seen from Fig. 7 (left column), the shapes of the high temperature region are all displayed as a cone. However, the maximum temperature level of the three cases has a significant difference, the maximum temperature (only 2291K) of the flame in the Case F is 17.6% lower when compared to the Case A. The amount of reactants for the homogeneous combustion in the Case F are lower than that of Case A, and the addition of final product can take the heat away in the chamber, indicating a decrease of maximum temperature level in the Case F. From Fig. 7 (right column), the high OH concentration region displays a cone shape. It can be noted that the maximum OH concentration level for the Case F is significantly lower than that of other cases. It is indicated that a mild reaction process can take place, even though hydrogen has a fast reaction rate. In addition, the temperature and OH concentration distributions in the Case F are very similar to that of Case D. Despite the fact that the intermediate can rapidly unite with hydrogen to form water, small amounts of intermediate also have a weak promotion effect on the homogeneous combustion. However, as mentioned above, the addition of final product can decrease the flame temperature and inhibit the homogenous combustion, this means the effects of final product play a dominant role in Case F.

Fig. 7. Computed contours of temperature (left column) and OH concentration distributions (right column) in the channel for Case A, B and F.

Fig. 8 shows the temperature and OH concentration profiles on the centerline of the channel. It can be seen from Fig. 8a that the temperature sharply increases and then slowly decreases along the distance from inlet to outlet in the three cases. For the Case F, the peak temperature position is far away from the inlet and the outlet temperature is 14% lower compared with Case A. Based on the above analysis, it can be concluded that the decreased reactants and the added final product can reduce the centerline temperature of the channel. It can also be found that the OH concentration first increases and then decreases sharply, as shown in Fig. 8b. Furthermore, OH concentration profiles have different peak values. The location of peak OH concentration in Case B significantly shift towards the inlet. The distance for Case A from the location of peak to the inlet is furthest, but the peak for Case F lies in the middle. This indicates that the products from the heterogeneous reactions should be shifted to the anchoring position of flame and alter the flame structure. The peak value of Case F is about 59.8% less as compared with the Case B and about 2.18 times less when compared to the Case A. The reduced reactants in Case F can sufficiently diffuse in the same bulk and then be induced, resulting in the

decrease of maximum OH concentration level. In Case B, the inhibition of heterogeneous reactions on the homogeneous combustion is mainly caused by the dominant position of final product effect. However, the maximum OH concentration level is still higher than that of Case F due to a high reaction rate of hydrogen in the oxygen. It is implied that the final product may be desorbed at the latter part of catalyst and then affects the post-flame zone of homogeneous combustion in the channel.

Fig. 8. Temperature (a) and OH concentration (b) profiles on the centerline of channel.

Fig. 9 shows the profiles of H_2O mass fraction and fuel conversion ratio on the centerline of the

channel. It can be seen that the mass fraction of H_2O first sharply increases and then increases slowly. It is worth noting that for the Case F, the mass fraction of H_2O sharply arrives at a higher value, and it is higher than that of other cases at the same place due to the addition of H_2O to reactants. The final product (H_2O) is desorbed from catalytic wall to the channel, resulting in an increase of mass fraction of H_2O in the channel. Fig. 9a shows the H_2 conversion ratio profiles on the centerline of the channel. At the upstream of the channel, the H_2 conversion ratio for Case B is higher than that of other cases. This indicates that the catalytic effects are more significant. As we know, a properly maintained high wall temperature in localized space can extend the gas reaction and mitigate radical quenching [13, 21]. In heterogeneous reaction for H_2/O_2 mixture, the heat formation and the desorbed intermediate can improve homogeneous reactions. In other words, the two factors interplay, resulting in a higher H_2 conversion ratio. As compared with the other cases, the H_2 conversion ratio for the Case F lies in the middle at the upstream part of the channel. The mean H_2 conversion ratio at the outlet is 0.986, 0.987, 0.988 for Case A, B and F, respectively. Even though the mean H_2 conversion ratios at the outlet for these cases have very little distinctions, the higher value for Case F indicates that the desorbed products have an effect on the homogeneous combustion. Therefore, the catalytic effects are more pronounced for the hetero-/homogeneous combustion system, which also include the effects of desorbed gaseous species from heterogeneous reactions.

Fig. 9. H₂O mass fraction (a) and fuel conversion ratio (b) profiles on the centerline of channel.

4. Conclusions

Two CFD models were carried out with detailed gas phase and catalytic chemical reaction mechanism of premixed H₂/O₂ mixture in the micro channels. The impacts of the desorbed products from heterogeneous reactions on the homogeneous combustion characteristics were studied using FLUENT. The simulation results demonstrate that the addition of intermediate can promote fuel

combustion efficiency and decrease the exhaust temperature. However, the intermediate desorbed from heterogeneous reactions shows a weak effect on homogeneous reactions due to a few amount of intermediate. In addition, with addition of final product, the gaseous temperature and fuel conversion ratio in the channel both significantly decrease because the addition of final product can take away the reaction heat and reduce the combustion intensity. As a result, the addition of final product mainly suppresses the homogeneous combustion. Furthermore, the inhibition of final product on the homogeneous combustion is still significant due to the dominant position of a larger proportion of final product in reactants. Hence, in the hetero-/homogeneous combustion system, the desorbed products from heterogeneous reactions have the suppression effect on homogeneous combustion, yet the ultimate effect for the system can generally promote the combustor performance, especially combustion efficiency.

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Table captions

Table 1 Mass fraction of gaseous species at the outlet gained by numerical simulation in first model.

Table 2 Inlet boundary conditions from different cases in the homogeneous reaction mode

Table 3 Fuel conversion ratio and mean outlet temperature for different cases.

Figure captions

Fig. 1. Schematic of the computational domain: Model 1 is 1mm in length and the inner wall is coated with platinum catalyst. Model 2 is 10 mm in length, and the catalyst segment is 1 mm length at the inlet in the inner surface.

Fig. 2. Centerline temperature profiles of combustor at a inlet flow rate of 26.4064 g/h with different mesh densities

Fig. 3. Comparison of centerline temperature profiles on the outer wall of experiment and simulation with non-/ catalytic wall.

Fig. 4. Computed contours of the OH concentration distributions (left column) and H₂O concentration distributions (right column) in the micro catalytic reactor.

Fig. 5. Computed contours of temperature (left column) and OH concentration distributions (right column) in the micro-reactor for Case B, C and E.

Fig. 6. Temperature (a) and OH concentration (b) profiles on the centerline of channel.

Fig. 7. Computed contours of temperature (left column) and OH concentration distributions (right column) in the channel for Case A, B and F.

Fig. 8. Temperature (a) and OH concentration (b) profiles on the centerline of channel.

Fig. 9. H₂O mass fraction (a) and fuel conversion ratio (b) profiles on the centerline of channel.