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Catalytic ignition of multi-fuels on platinum: effect of strain rate

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Abstract

Numerical simulation of the catalytic ignition of multi-fuels is performed in a stagnation flow to identify the interaction among the primary components of gasified biomass on platinum surface. Simulations of selected single fuel are firstly performed and the results are compared with available experimental data. The results show that the ignition temperature increases with strain rates for the major biomass components as they are catalytically ignited individually. For H_2/CO mixture, the two components always ignite simultaneously and the existence of H_2 in the mixture will result in a lower ignition temperature than that for the sole CO. On the other hand, catalytic combustion of H_2 or CO would help to reduce the catalytic ignition temperature of CH_4 in the H_2/CH_4 or CO/CH_4 mixture. However, the ignition for the synthesized gasified biomass would depend on the fuel concentrations and the strain rate. The existence of other components in the simultaneous multi-fuels and the competitions between different fuels and oxygen for active surface sites change the catalytic ignition behavior. Higher strain rate would result in higher steady-state surface temperature, but it would also require higher ignition temperature. These phenomena can be explained by the characteristics of the surface coverage of the main surface species.

Keywords: Catalytic ignition; Strain rate; Multi-fuels

1. Introduction

In view of its capability of burning different fuels with high efficiency at a relatively low temperature and under lean conditions, catalytic combustion technique has been identified as one of the most promising methods for clean and high-efficiency combustion in the new century. Furthermore, catalytic combustion of gasified biomass has been seriously considered for clean and effective usage of this renewable energy. Gasified biomass includes many gaseous fuel components, mainly H_2, CO and CH_4. Its practical application is determined by the interaction of these major components and affected by many factors. Among these factors, the catalytic ignition of the gasified biomass on the catalyst surface stands among the outstanding issues, as it is a major concern associated with the design and operation of a catalytic combustor. So far, most reported works on catalytic combustion of gasified biomass have focused on the circumventing fuel-NO_x formation, H_2O effect and conversion ratio with different catalysts. Spherical pellet catalyst or monolith honeycomb catalyst were commonly used for practical applications [1–3]. Catalytic ignition of single hydrocarbon fuel on platinum catalysts has been investigated in the literature and the results actually showed different ignition behaviors [4–8]. The ignition temperature for hydrogen and carbon monoxide increases with increasing fuel concentration, while that for methane decreases with

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increasing methane concentration. On the other hand, as reported in some preliminary test results the catalytic ignition characteristics for multi-fuels including gasified biomass would be completely different from that for each individual fuel. These results are contradictory to the conventional concept of using a fuel with a low ignition temperature to raise the catalyst surface temperature and help to ignite the fuel with a higher ignition temperature [9]. The existence of other components in the simultaneous multi-fuels and the competitions between different fuel components and oxygen for active surface sites would change the catalytic ignition behaviors.

Stagnation flow is often used to investigate the catalytic combustion characteristics as it is amenable to numerical analysis and is easier for instrument access to locations near the catalytic surface for measurements of the chemical activities [4–13]. By confining attention to the center of the surface, edge effects can be neglected and the scalar quantities depend only on the distance from the surface and not on the radial position, permitting use of one-dimensional analysis. Although it is easy to identify catalytic ignition for single fuel by an abrupt rise of surface temperature, the condition is not the same for multi-fuels and information of surface coverage would be needed. So, in this work, in order to gain more insight into the interaction of primary components on the catalyst, numerical simulation of catalytic ignition of multi-fuels including synthetic gasified biomass at atmospheric pressure is performed in a stagnation flow over platinum surface with detailed reaction mechanism. Moreover, it has been found that the flow straining has a direct effect on catalytic ignition. The strain rate effect has been extensively investigated for gas phase combustion but it was less discussed for catalytic combustion. Therefore, the strain rate effects on the catalytic combustion and ignition process are also studied in this work.

2. Numerical method

The stagnation flow field is shown schematically in Fig. 1. In this work, numerical simulation for the stagnation flow with gas phase and surface reactions is performed. The numerical model used to simulate the catalytic combustion consists of the coupling of the flow field and the chemical reactions in the gas phase and on the catalyst surface. The computational solution is accomplished by using the program SPIN, which uses the TWOPNT software, which implements a Newton/time-step algorithm [14,15]. The details of the governing equations and the solution methods can be found in the users' manual. The surface temperature of the catalyst could be increased by stepwise increasing the power applied to the catalyst or by preheating the mixture. After each increment of power or preheating temperature of the mixture, the system is allowed to evolve to a new steady state. When approaching the ignition point, the Newton iteration may

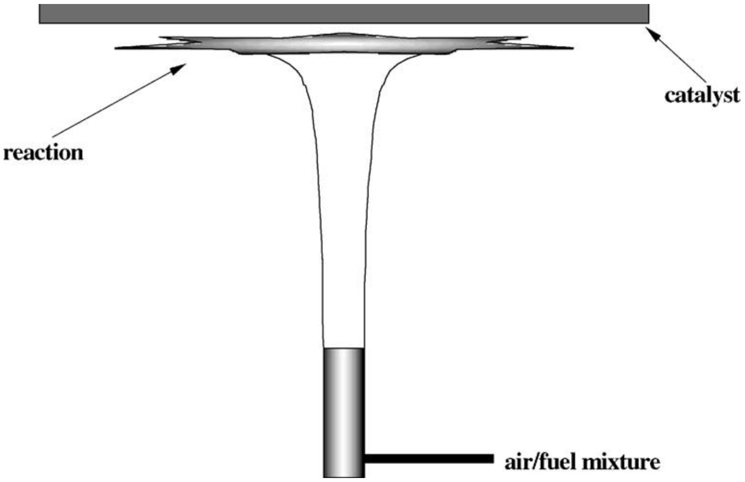

Fig. 1. Schematic diagram of the stagnation point flow.

Table 1
Surface reaction mechanism on Platinum catalysts

Reactions	*A*	S_0	*b*	E_a
Reactant adsorption/desorption				
1. CO + PT(*) ⇒ CO(*) + PT(B)		0.84	0.0	0.00
2. CO(*) + PT(B) ⇒ CO + PT(*)	1.0E+13		0.0	126.0
3. H_2 + 2PT(*) ⇒ H(*) + H(*) + 2PT(B)		0.046	0.0	0.00
4. 2H(*) + 2PT(B) ⇒ H_2 + 2PT(*)	3.7E+21		0.0	67.4-11H(*)
5. CH_4 + 2PT(*) ⇒ CH_3(*) + H(*) + 2PT(B)		0.01	0.0	0.00
6. O_2 + 2PT(*) ⇒ 2O(*) + 2PT(B)		0.023	0.0	0.00
7. 2O(*) + 2PT(B) ⇒ O_2 + 2PT(*)	3.7E+21		0.0	216-60O(*)
Surface reactions				
8. H(*) + O(*) + PT(B) = OH(*) + PT(*)	3.7E+21		0.0	10.50
9. H(*) + OH(*) + PT(B) = H_2O(*) + PT(*)	3.7E+21		0.0	17.40
10. 2OH(*) = H_2O(*) + O(*)	3.7E+21		0.0	51.25
11. CO(*) + PT(*) ⇒ C(*) + O(*) + PT(B)	1.0E+18		0.0	156.5
12. CO(*) + O(*) + 2PT(B) ⇒ CO_2 + 2PT(*)	6.0E+18		0.0	49.14
13. C(*) + O(*) + PT(B) ⇒ CO(*) + PT(*)	3.7E+21		0.0	62.5
14. CH_3(*) + PT(*) ⇒ CH_2(*) + H(*) + PT(B)	3.7E+21		0.0	20.0
15. CH_2(*) + PT(*) ⇒ CH(*) + H(*) + PT(B)	3.7E+21		0.0	20.0
16. CH(*) + PT(*) ⇒ C(*) + H(*) + PT(B)	3.7E+21		0.0	20.0
Product adsorption/desorption				
17. H + PT(*) ⇒ H(*) + PT(B)		1.000	0.0	0.00
18. O + PT(*) ⇒ O(*) + PT(B)		1.000	0.0	0.00
19. OH + PT(*) ⇒ OH(*) + PT(B)		1.000	0.0	0.00
20. OH(*) + PT(B) ⇒ OH + PT(*)	1.0E+13		0.0	192.80
21. H_2O + PT(*) ⇒ H_2O(*) + PT(B)		0.7500	0.0	0.00
22. H_2O(*) + PT(B) ⇒ H_2O + PT(*)	1.0E+13		0.0	45.5

be difficult to converge and instead, the transient problem is solved till the steady state is established.

The chemical mechanisms are used in the gas phase and on the surface. The reaction rate is represented by the modified Arrhenius expression and for the surface chemistry, all temperature exponents are set to zero. The gas phase reaction mechanism is adopted from literatures without any modification [16,17]. Due to the fuel lean conditions for both single fuel and multi-fuels, the preliminary calculations without gas reaction model did not show obvious differences. Many reports in the literature also showed that the surface temperature required for gas phase ignition was higher for catalytic than for noncatalytic surface. In other words, the homogeneous ignition was inhibited by the catalyst, especially for lean conditions [5,12]. The surface reactions shown in Table 1 have been compiled primarily from literatures without adding any reaction step and have been tuned to model catalytic ignition of single fuel and multi-fuels cases [4,6–8,18]. Ten surface species (H(*), O(*), OH(*), H_2O(*), C(*), CO(*), CH_3(*), CH_2(*), CH(*), Pt(*)) describe the coverage of the surface with adsorbed species. Pt(*) denotes the free surface site which is available for adsorption. The Chemkin software for gas phase chemical kinetics, and Surface Chemkin for heterogeneous chemical kinetics are used in this study and the details of the chemical reaction rate formulation can be found in the users' manual.

3. Results and discussion

In the study, the inlet mixture consists of 2.7% hydrogen, 3.6% carbon monoxide and 1.1% methane, 16% oxygen and nitrogen for the rest. The percentages of the ingredients are adopted according to the gasified biomass reported in the literatures [19,20]. However, it should be mentioned that the percentage of each ingredient would be different for different sources of biomass. With these concentrations, through several preliminary calculations, the results identify the reaction occurs primarily on the surface, not in the bulk gas phase. The global strain rate is defined as the inlet velocity divided by the separation distance, which is the distance between the catalyst surface and the jet exit. The global strain rate can be varied by either changing velocity or changing separation distance and both operations yield the same results.

3.1. Catalytic ignition for single fuel

Unlike the gas phase ignition, a prerequisite for catalytic ignition is the availability of a sufficient number of uncovered active sites on the catalyst. Therefore, the sensitivity analysis is often used to study the influence of rate coefficients on the number of the active surface sites. The sensitivity coefficients are given for H_2, CO and CH_4 oxidation on platinum immediately before ignition takes place (not shown here). Since the system is controlled by kinetics before catalytic ignition and ignition occurs when both fuel and oxygen can adsorb to the surface, the adsorption/desorption processes of reactant would determine the ignition process. For hydrogen and carbon monoxide, the desorption of fuel would be the critical step while for methane, oxygen desorption step is the key. These results indicate that the rate coefficients of these rate-limiting steps need to be carefully determined.

Firstly, simulations of single fuel ignition under different preheat temperatures are performed and the results are compared with available wire experimental data to further tune the surface reaction mechanism [4,5]. To determine the catalytic ignition temperature, simulations of cases of the reactive mixture flowing at atmospheric pressure on a catalytic wire or in stagnation flow toward a catalytic foil, which are identical to the experimental conditions of Cho and Law [4] and Griffin and Pfefferle [5], are performed. In their experiments, velocities in the range of 3–10 cm/s were used, corresponding to $Re < 1$. Due to the existence of axisymmetry, the catalyst wire can be essentially considered as being immersed in a constant concentration bath. Catalytic ignition temperatures for a stagnation point flow of H_2, CO and CH_4 in lean conditions are shown in Fig. 2. Comparisons of the numerical results with experimental data are satisfactory and the results show different ignition behaviors for different fuels. Among these fuels, H_2 is the easiest fuel to ignite and the ignition temperature is around 350 K. The ignition temperature for CO is around 650 K. CH_4 is the most difficult one to ignite and the ignition temperature is above 850 K. For the H_2/air and CO/air cases, the ignition temperature increases with increasing fuel concentration, however, for the CH_4/air cases the ignition temperature decreases with increasing fuel concentrations. These different ignition behaviors can be explained by examining the sticking tendency between different fuels and oxygen. Since the adsorption rate depends on the gas phase concentration, higher fuel concentration in the bulk gas leads to fewer active sites and that is responsible for the increase of ignition temperature in increasing H_2 and CO concentrations. In the CH_4/air system, the catalytic ignition is also connected with the adsorption/desorption kinetics. However, in this case, before ignition the main species on the surface is the oxygen causing an inverse dependence of the ignition temperature on fuel/oxygen ratio.

As for the strain rate effect, Fig. 3 shows the catalytic ignition characteristics for a stagnation point flow of single fuel/air system on a platinum surface with different strain rates. The preheated mixture impinges on the platinum surface. Before ignition, the system is kinetically controlled and the heat produced by surface reaction is unable to balance the heat loss due to fluid convection and thermal radiation for a self-sustained reaction. When reaching the ignition temperature T_{ig}, the temperature of the catalyst surface rises rapidly because of the heat release by the exothermic surface reactions. The results show that the ignition temperature increases with strain rates due to the increase of heat convection for these major biomass components as they are catalytically ignited individually, while the increment for hydrogen is slim. Due to higher heat convection induced by higher strain rate, less chemical heat release by surface reactions is remained to promote ignition. Higher preheat temperature is then needed for ignition. Figs. 4–6 show the catalytic ignition characteristics, in terms of surface temperature, fuel concentration, and surface coverage, as functions of preheat temperature and strain rate for different cases of single fuel/air mixture. In general, ignition on the surface is usually identified by the sudden jump of the surface temperature accompanied by sudden drop of the fuel concentrations and the surface coverage of the active surface species on the surface. However, for the methane/air system, there is no obvious sudden jump of the surface temperature when it is

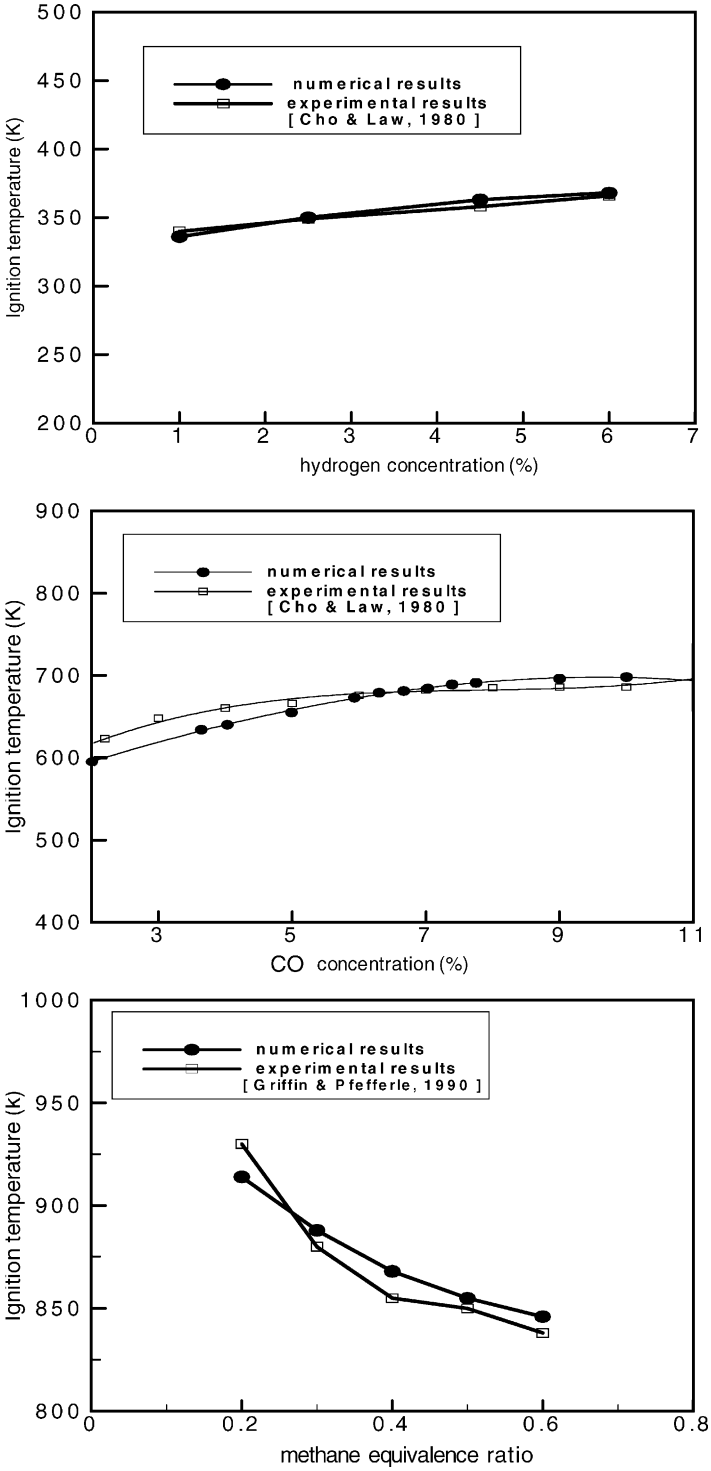

Fig. 2. Comparison of the numerical results with experimental data of catalytic ignition temperature on platinum wire.

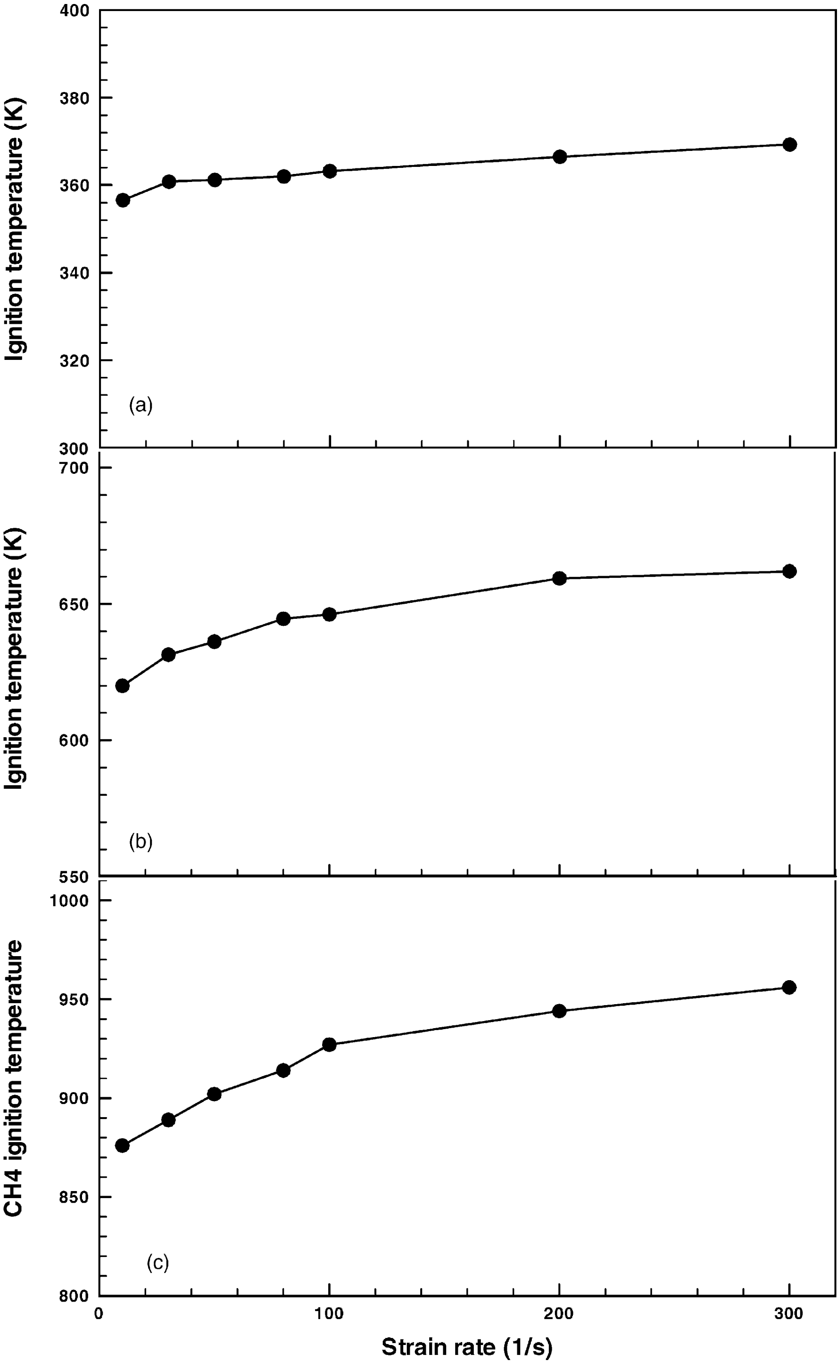

Fig. 3. Ignition temperature of single fuel/air mixture as a function of global strain rate: (a) 2.7% H_2; (b) 3.6% CO; (c) 1.1% CH_4.

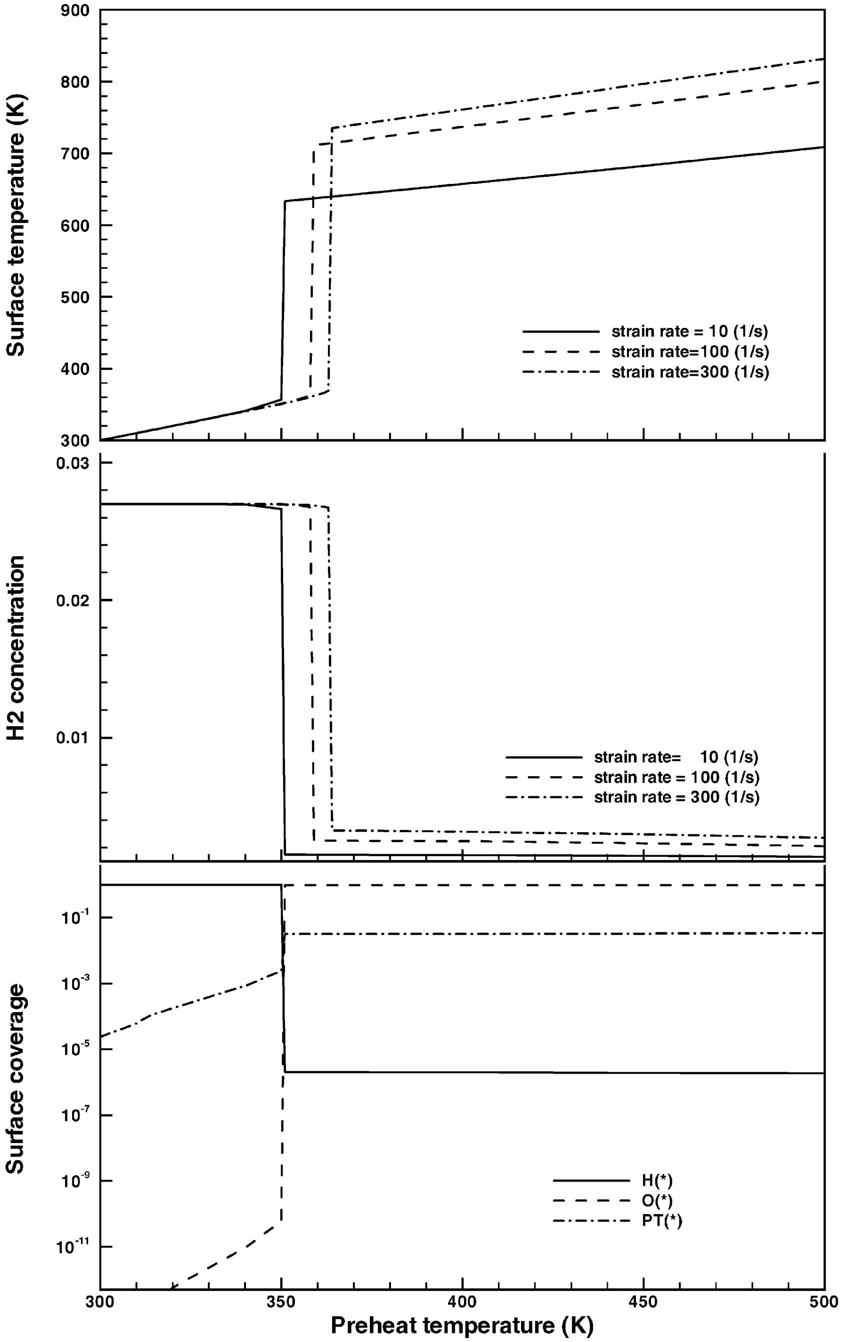

Fig. 4. The relation between the preheated temperature and surface temperature, fuel concentration and surface coverage of main species of 2.7% H_2 in air.

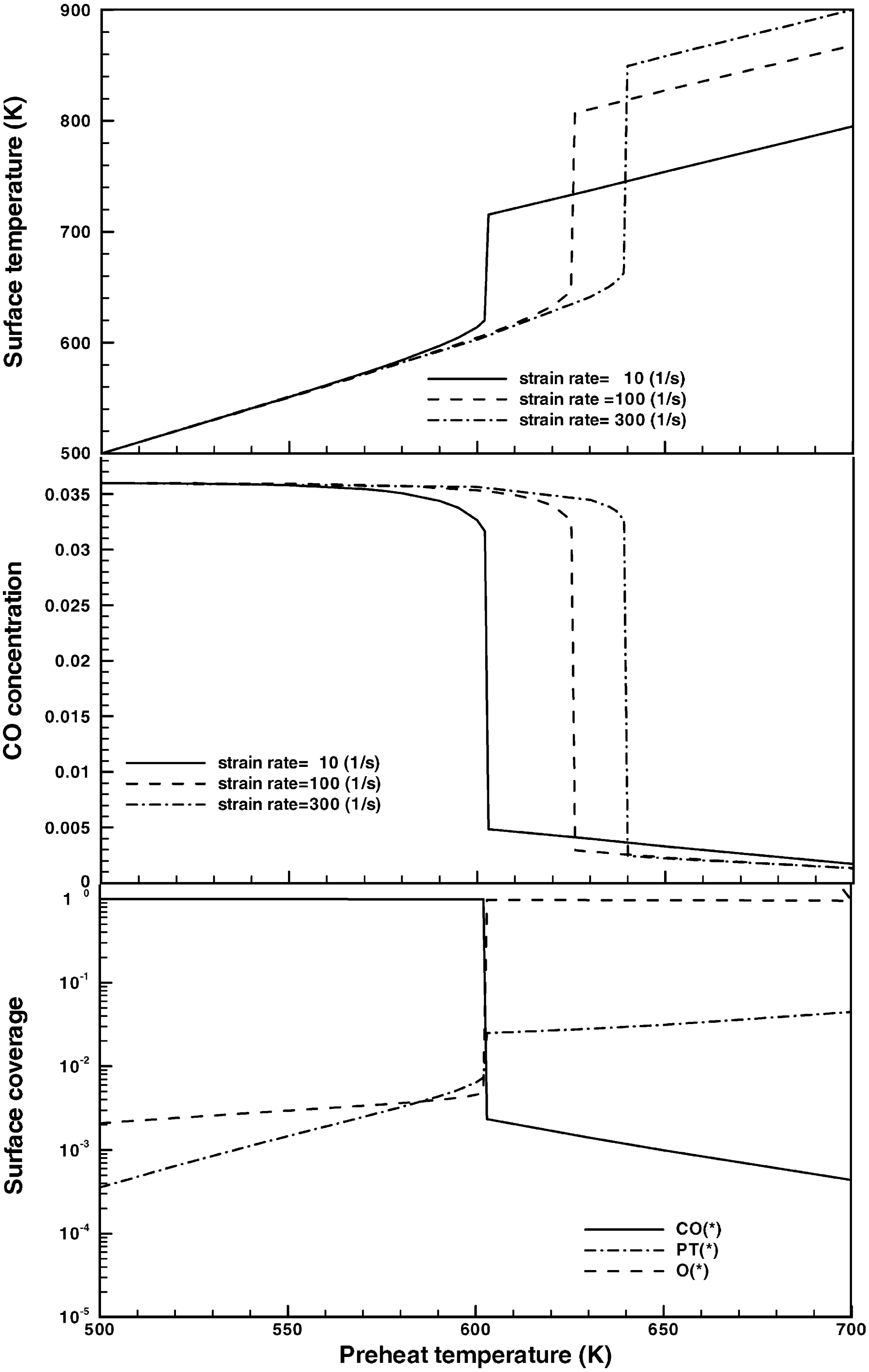

Fig. 5. The relation between the preheated temperature and surface temperature, fuel concentration and surface coverage of main species of 3.6% CO in air.

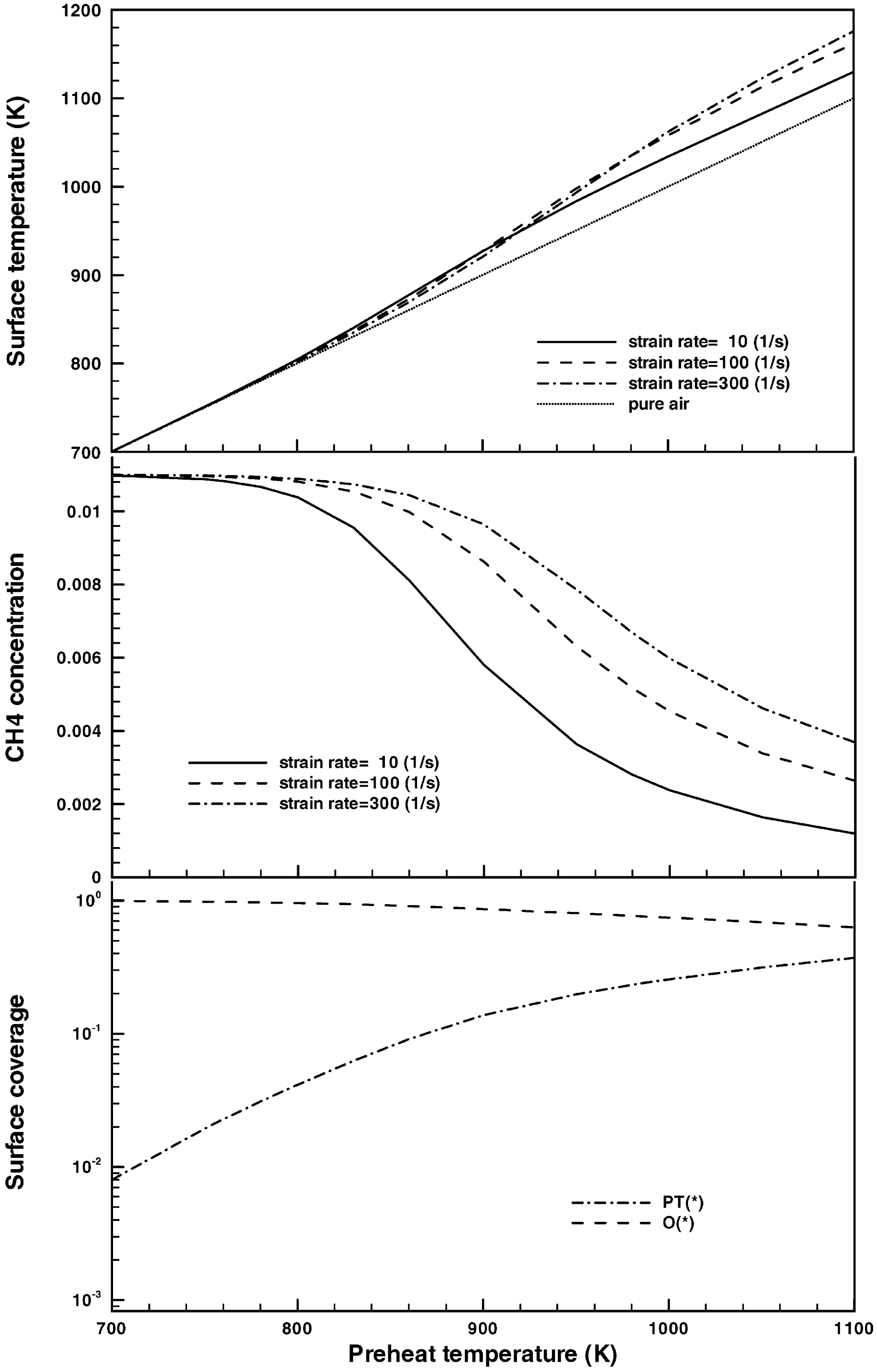

Fig. 6. The relation between the preheated temperature and surface temperature, fuel concentration and surface coverage of main species of 1.1% CH_4 in air.

ignited on the surface due to heat loss and low initial fuel concentration on the surface. The ignition temperature can then be determined from the variation of the CH_4 concentration and can be defined arbitrarily as the surface temperature where surface fuel conversion ratio reaches 50% of the reactants. Furthermore, higher strain rates shift the ignition curves towards higher preheat temperature. The results also show that higher strain rates result in higher steady-state surface temperatures and the temperature would exceed the adiabatic temperature for H_2 due to its high diffusivity.

The surface coverage of main species in Figs. 4–6 shows that before ignition the catalyst surface is almost completely covered by fuel for the H_2/air and CO/air cases. This is because H_2 and CO have higher adsorption ability to the catalyst surface than oxygen. As the surface temperature is increased, the desorption of fuels is enhanced yielding more bare surface sites for oxygen to adsorb. Then, H(*) can react immediately with the surrounding O(*) to form OH(*) and this leads to relatively fast formation of H_2O on the surface, which is then desorbed into gas phase. Similarly, the adsorbed CO(*) reacts with O(*) to form CO_2. For CH_4, the surface is almost completely covered by oxygen before ignition. An increase of the preheat temperature leads to a point at which the adsorption/desorption equilibrium for oxygen shifts towards desorption, resulting in active sites for CH_4 adsorption to induce further reaction and the product is then desorbed. So more and more active sites become available for CH_4 adsorption and for further O_2 desorption. The chemical heat accelerates the reaction rate to cause ignition. Since it is in fuel lean condition, the surface is almost covered by oxygen after ignition. In addition, the energy balance at the surface requires estimating the radiation losses from the surface, which in turn, requires an estimate of the emissivity of platinum. In this study, an emissivity 0.3 is used when the surface is covered with oxygen as proposed by Warnatz et al. [7].

The temperature and fuel concentration profiles for single fuel with different global strain rates are shown in Fig. 7. The resultant temperature profiles imply that the system is dominated by surface reactions. After ignition, the system transits from kinetic control to mass-diffusion control. The mass diffusion is faster at high strain rates and the fuel in the bulk gas mixture takes less time to reach the surface. Consequently, more fuel is consumed on the surface and thus more heat is generated to raise the catalyst surface temperature resulting in higher steady-state surface temperatures as shown previously in Figs. 4–6. However, the heat loss, which would reduce reaction, also increases with increasing strain rates. It is these two competing factors that affect the fuel conversion on the surface.

3.2. Catalytic ignition for multi-fuels

To further investigate the complicated interactions of different fuel species on the catalytic surface, numerical studies of the multi-fuel cases are then performed. The multi-fuel results show complete different behaviors from the single fuel cases because of the competition of the simultaneous multi-fuel and oxygen for active sites on the surface. First, the ignition characteristics of H_2/CO/air mixture are shown in Fig. 8. Compared with the results in Fig. 4, hydrogen cannot be ignited at low temperature anymore. The predicted fuel concentration versus the preheated temperature shows that H_2 and CO almost ignite at the same preheated temperature. It is obvious that hydrogen ignition is affected by the presence of carbon monoxide. It is not surprising since CO adsorbs more easily to the catalyst surface than H_2. Strain rate effect is also obvious in the H_2/CO/air mixture case. The preheated temperature for simultaneous ignition of H_2/CO/air mixture (586–621 K) is much higher than that for H_2/air ignition (351–364 K), but is lower than that for CO/air ignition (603–640 K). In other words, H_2 ignition is delayed due to the presence of CO and CO ignition is enhanced due to the presence of H_2. The relation between the preheated temperature and surface coverage of primary species helps to explain this observation. Before ignition, the catalyst surface is almost occupied by carbon monoxide, while the hydrogen is also adsorbed on the surface to some extent. When the preheated temperature is increased, CO begins to desorb and more active sites are available. At these temperatures, the adsorption/desorption equilibrium of hydrogen shifts to desorption and most active sites are available for oxygen adsorption. The adsorbed O(*) would then react with H(*) and CO(*) and simultaneous ignition occurs.

Fig. 9 shows the ignition characteristics of H_2/CH_4/air mixture. The H_2 ignition is not affected by the presence of methane and the preheated

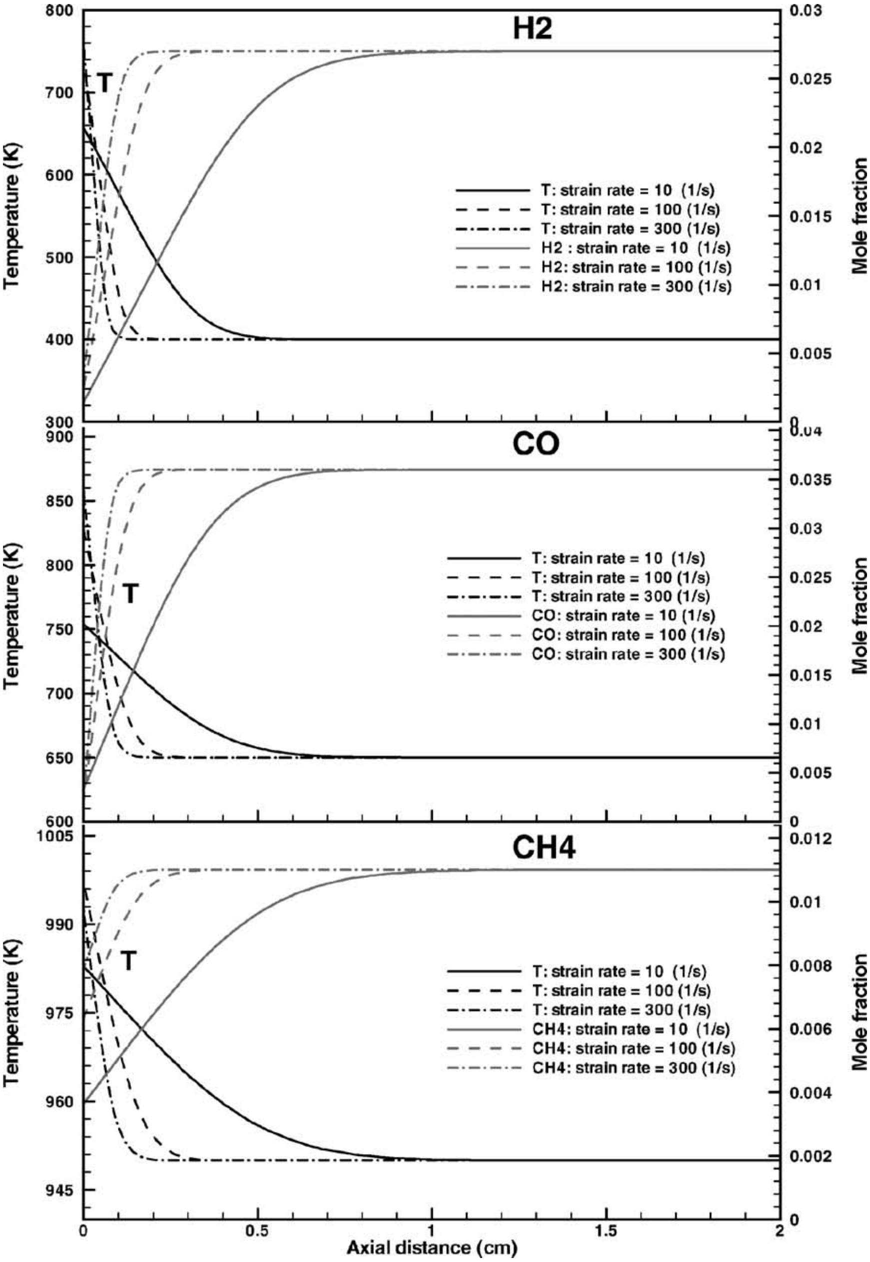

Fig. 7. The temperature and fuel concentration profiles of single fuel in air with different global strain rates at the preheated temperature 400, 650 and 950 K, respectively.

temperature for H_2 ignition is almost the same, as hydrogen has higher adsorption ability to the surface than methane. Initially, the catalyst surface is almost completely occupied by hydrogen before ignition. As the H_2 ignition temperature is reached, the surface temperature rises rapidly but the CH_4 does not ignite simultaneously as shown in the relation between the preheated temperature and the CH_4 concentration.

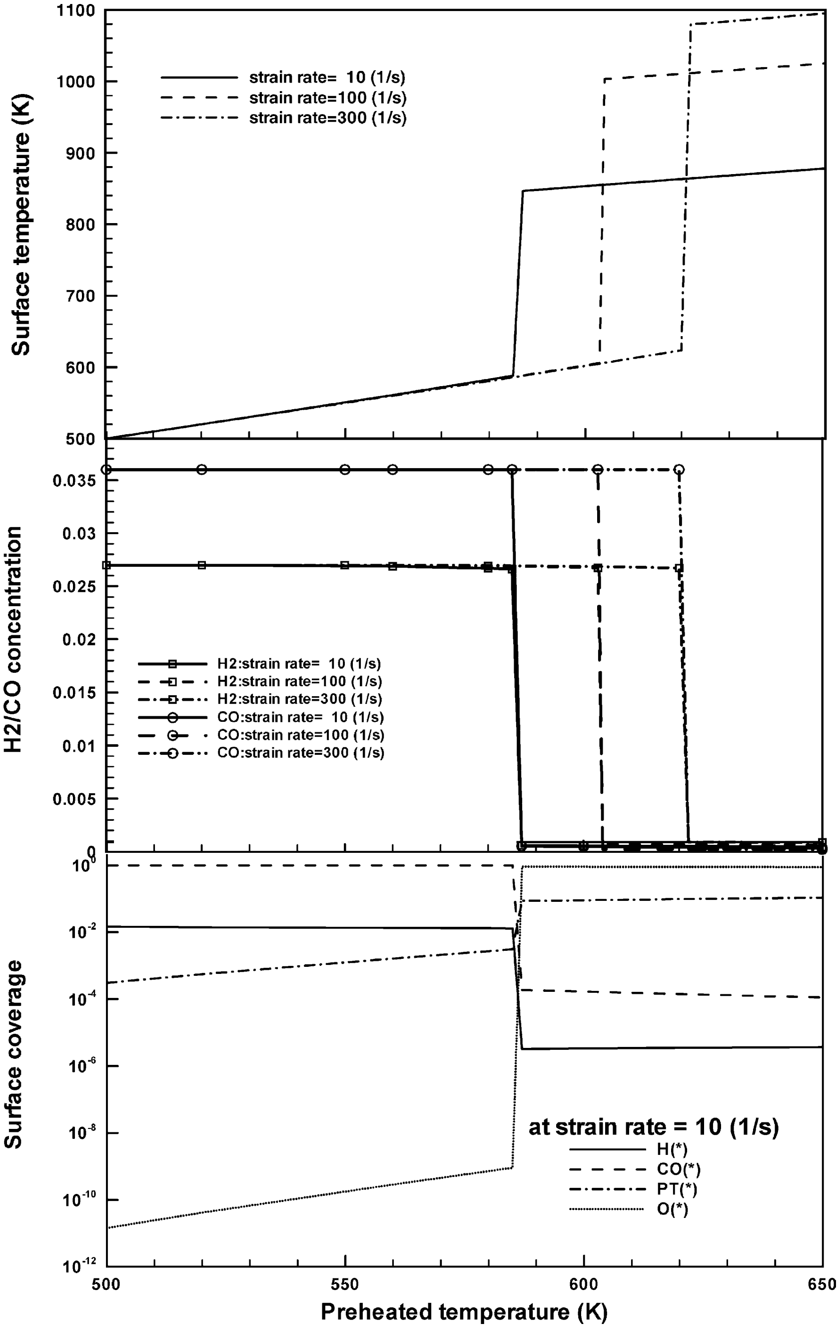

Fig. 8. The relation between the preheated temperature and surface temperature, fuel concentration and surface coverage of main species of 2.7% H_2 and 3.6% CO in air.

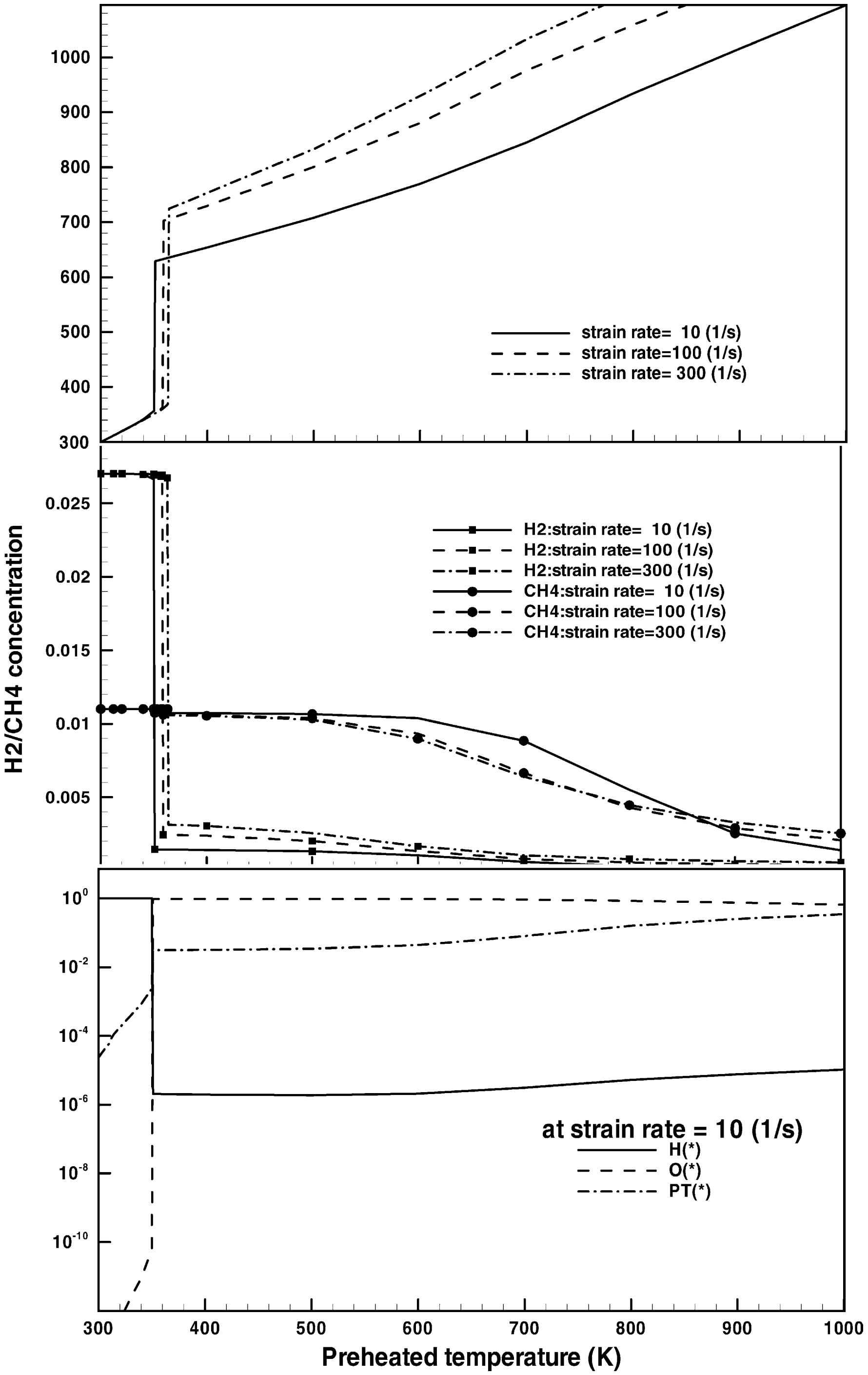

Fig. 9. The relation between the preheated temperature and surface temperature, fuel concentration and surface coverage of main species of 2.7% H_2 and 1.1% CH_4 in air.

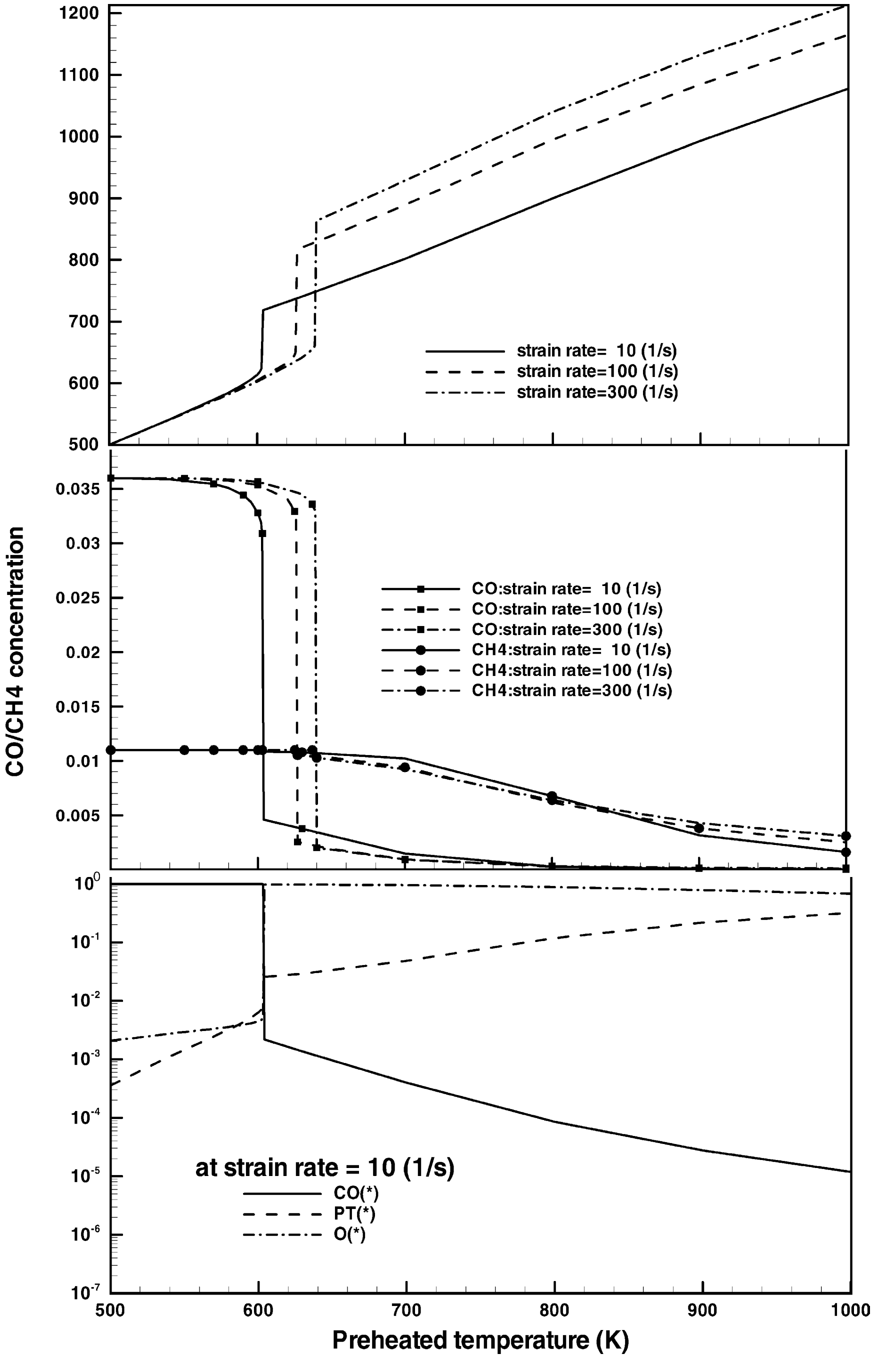

Fig. 10. The relation between the preheated temperature and surface temperature, fuel concentration and surface coverage of main species of 3.6% CO and 1.1% CH_4 in air.

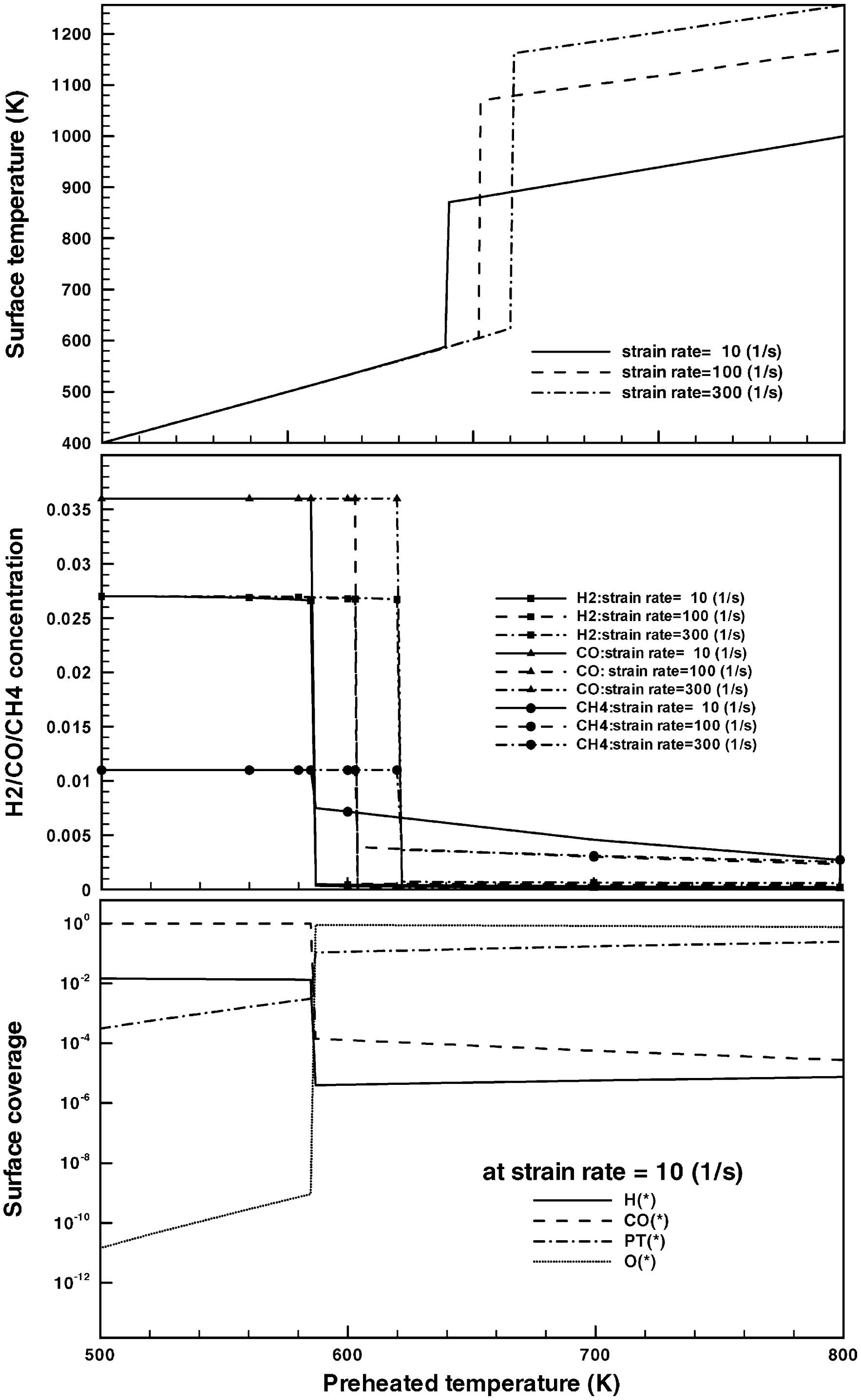

Fig. 11. The relation between the preheated temperature and surface temperature, fuel concentration and surface coverage of main species of 2.7% H_2, 3.6% CO and 1.1% CH_4 in air.

The heat release by H_2 oxidation does not raise the surface temperature sufficiently high for the catalytic ignition of CH_4. However, the catalytic reaction of H_2 still helps to reduce the preheated temperature for CH_4 ignition. In addition, strain rate effect produces inverse results for CH_4 ignition. Higher strain rate results in higher steady-state surface temperature after H_2 ignition. Although higher strain rate results in a higher ignition temperature for methane, the difference of the preheated temperatures between H_2 and CH_4 ignition is reduced with strain rate.

Additionally, the ignition characteristics of CO/CH_4/air mixture are shown in Fig. 10. Again, the CO ignition is almost not affected by methane since CO has the highest adsorption probability (sticking coefficient) among these fuels and oxygen with respect to the platinum catalyst. The catalyst surface is almost completely occupied by carbon monoxide before ignition and the preheated temperatures for CO ignition are almost the same as those in the single fuel cases. The heat release by CO oxidation also does not raise the surface temperature high enough to induce CH_4 ignition. The surface coverage profiles indicate that after CO ignition, the active sites are almost completely occupied by oxygen and CH_4 cannot adsorb to precede further reactions. The increase of the preheating temperature will enhance oxygen desorption and more active sites will be available for CH_4 adsorption. The strain rate effect is also obvious. Higher strain rate results in higher steady-state surface temperature after CO ignition and then CH_4 can ignition at a lower preheating temperature. In other words, higher strain rates make simultaneous ignition prevailing.

Then, catalytic ignition of the synthetic gasified biomass (H_2/CO/CH_4) is performed and the results are shown in Fig. 11. Similar to the H_2/CO/air case, before ignition the surface is covered primarily by carbon monoxide and by hydrogen to some extent. Increasing the preheating temperature results in free surface sites for oxygen adsorption. But at this time, the simultaneous ignition of H_2 and CO also ignites methane for different strain rates. This is shown in the relation between the preheating temperature and the fuel concentration, where all three fuel concentrations have a rapid drop at the same preheating temperature. Comparing with the results of H_2/CO/air and CO/CH_4/air cases, it is evident that the chemical heat release by CO and H_2 oxidation is sufficient to raise the surface temperature to reach the ignition temperature of methane. In other words, the fuel concentration is also an important factor that affects simultaneous ignition of methane with hydrogen and carbon monoxide. Therefore, in gasified biomass, hydrogen and carbon monoxide always ignite simultaneously while methane is not. Obviously, the percentage of each ingredient in gasified biomass would be different due to different sources and it will affect the ignition characteristics. Higher percentage of hydrogen and carbon monoxide will release more chemical heat to enhance methane ignition but a lower methane concentration needs higher ignition temperature. In a practical system like a monolithic honeycomb reactor, it is an important factor related to the steady-state operation. Finally, in this study, although direct experimental verification is not available yet and related literatures are scarce, the above ignition characteristics for multi-fuels are also experimentally found in the platinum honeycomb reactor (prepare to be published soon). Since ignition processes are determined by the competitions between reactant adsorption and desorption, it is believed that the ignition characteristics will remain the same in either honeycomb or stagnation point flow geometry.

4. Conclusions

In this study, the catalytic ignition characteristics of single fuel, multi-fuel and synthetic gasified biomass cases are performed numerically in the stagnation point flow over platinum. The existence of other components in the simultaneous multi-fuels and the competition between different fuels and oxygen for active surface sites change the catalytic ignition behavior. Higher strain rates would result in higher steady-state surface temperature, which is due to the faster mass diffusion, but it would also require higher ignition temperature due to higher heat loss. The competition of these two factors determines simultaneous ignition. Hydrogen ignition is delayed by the presence of CO, while CO ignition is enhanced by H_2 in the multi-fuel cases. They always ignite simultaneously. Among the three fuels, methane is the most difficult one to ignite and the ignition can be enhanced by the co-presence of hydrogen and carbon monoxide in the gasified biomass. Higher strain rate would promote simultaneous ignition in the cases considered. Since the ignition temperature of single fuel is dependent on the fuel concentration, the percentage of each ingredient in multi-fuel or gasified biomass would also determine simultaneous ignition. Finally, these phenomena can be explained by the characteristics of the surface coverage of main species.

Acknowledgements

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