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Utilisation of H₂O and CO₂ in Coal Particle Gasification with an Impact of Temperature and Particle Size

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Abstract

Aiming at improving the quality of syngas, the thermochemical behaviour of syngas formation during a single coal particle gasification process is investigated based on a validated numerical model. Initially, simulations of coal gasification with steam (H₂O) are conducted in a reactor, and the results show that the steam gasification generally favours the production of H₂ and CH₄. However, a switch of agent to CO₂ into the gasifier influences the gasification products having H₂, CO and CH₄. This is then prompted to the investigation of a mixture of H₂O and CO₂ agent in the reactor's environment, and the results show a promising indicator in producing the overall better syngas quality. Moreover, the influence of the coal particle size and gasification temperature on the syngas production is studied. The results

identify that the concentration of syngas products is higher when using smaller coal particles as the behaviour of heterogeneous reactions of CO formation is affected by the particle size. Finally, high temperature promoted the chemical reactions of the gasification process, resulting in the improved production of syngas.

Keywords: Thermochemical process, syngas products, coal particle gasification, CO₂ and H₂O utilisation, Computational Fluid Dynamics.

1 Introduction

The coal reserve is abundant, and its price is cheaper than oil and natural gas as an energy source. The total amount, including the economically non-recoverable, is reported to be 18 terratons, and most of them are too deep or too costly to be mined by traditional methods [1-3]. The coal will still be the largest fuel sources for the electricity generation until 2040 as it is predicted in Ref. [3]. Therefore, improving coal utilisations is still an important topic and research is continuously conducted.

However, the environmental issue has become a major concern on coal utilisation. The high level of carbon dioxide (CO_2), and other unwanted gases (such as H_2 , Tar, H_2S , etc.) from coal combustion are exhausted into the environment. Hence, Clean Coal Technology (CCT) was introduced, with an aim to provide the technology of coal utilisation that could provide an environmentally satisfactory and economically viable solution [4]. The CCT has been developed since 2000, and now is still relevant with more advances on the development. The CCT covers a wide range of areas, from the coal production up to utilisation, and coal gasification is one of the development technologies at the utilisation stage. Coal gasification is a part of coal conversion technologies which include all kinds of chemical conversion pathways for coal beside combustion [5]. Further process of coal gasification results in chemical raw material or other forms of fuel. And, the development of coal gasification not only limits in the coal utilisation from the ground surface, but also includes coal resources from the deep underground.

Figure 1 presents the gasification processes of coal. Initially, the moisture evaporates, then the coal's volatile matter (VM) releases during the devolatilization process. Afterwards, the VM (consisting of C, H, O, and N) and char react with oxygen in the oxidation zone and the produced gaseous species are shown in the figure. Most of the oxygen is consumed in the

oxidation zone, and when the chemical reactions take place in the absence of oxygen or at extremely low oxygen concentrations, the reduction reactions as well as pyrolysis occur. The syngas is the final result. As also clearly identified in Figure 1, the reaction mechanisms of coal gasification, irrespective of the scaling of the model, are essentially the same [6, 7]. Therefore, this study offers the scale of particle level of coal gasification. The proposed particle based computational model provides an opportunity to investigate the fundamental aspects of the thermochemical process physics which usually occur in gasification. This also provides the flexibility to identify the effects of various relevant operating and boundary conditions on gasification.

The study of coal particle gasification has been initiated with the focus on the investigation of kinetic parameter. It has been validated at the stage of oxidation reactions with the coal particle combustion experimental test. The detailed study can be seen in the publication cited in Ref. [8]. The current study is an extension of the previous one, and particularly focuses on the process of investigation to improve the syngas products in the gasification process. Several investigations to improve the syngas quality have been conducted, such as with steam (H_2O) addition [9-12], and through of a review of CO_2 conversion as considered in the *Boudouard* reactions [13]. These references [9-12] provided the information of the effect of H_2O addition based on the experimental results, whereas the current study develops the numerical simulation approaches. The results of both methods can be compared. Meanwhile, the literature for CO_2 addition in process of gasification [13], focused only on the char reactions as presented by the *Boudouard* reactions. The current study uses more detailed reactions that involve the gasification kinetics (see Table 1). Therefore, it is more reliable to be applied into the numerical simulation approach. Additionally, the study considers the effect of other parameters such as temperature and seam coal strata, as conducted by *Yang et al.* [14, 15], and *Younger* [16]. They described the effect of temperature into the physical properties or behaviour of coal seam. This study incorporates the information with focus on

the thermochemical behaviour of the gasification reactions, leading to the improved quality of syngas production.

Furthermore, the coal particle gasification model is suitable to simulate the process, as the single particle model is able to present the reaction mechanisms [8]. Other methods, such as surface reaction has limitation to provide multiphase reactions, and coal block method has limitation in providing radiation reactions [8]. Moreover, by conducting the gasification simulation in the particle level, the behaviours of chemical reactions can be clearly presented and identified with more details.

Finally, this study is expected to provide an indepth understanding of the thermochemical behaviour during the gasification process with the reaction mechanisms sourced from the several studies [17, 18]. It can be considered further to improve the quality of gasification products.

2 A brief overview of the numerical model

The developed numerical model for gasification simulation was described and validated in detail in the previous publication [8, 19-22]. Here, a brief summary of the model is given in this section to provide the sufficient information for understanding the simulation process.

Figure 2 illustrates the schematic of the gasifier with the axisymmetric model grid. A procedure of directed/structured mesh is used, with the cells concentrated at the centreline. At this area, the coal reaction zone is located and, as a result, large gradients in flow properties exist. Therefore, more cells are concentrated here to provide better accuracy in resolving the gradients. The state of mass and species in the gasification simulation changes over time and is governed by the equations of state. They consist of the equations of continuity, momentum, chemical species transport, and conservation of energy [20, 23, 24]. The governing equations used in the numerical procedures can be seen in Sutardi et al. [8].

An implicit unsteady model is used that coupled with the segregated flow, fluid energy and species models for the simulations. This model allows the simulation of the object based on the iteration of time-step. The second-order accurate scheme is used for discretization, with the criterion of convergence being set to 10^{-6} for the equations of energy and radiation, while 10^{-4} for the other transport equations.

Gaseous chemical reactions are defined as in Ref. [8, 17] and Eddy Break Up (EBU) model with the kinetic control parameter implemented to control the reaction mechanisms [25]. The kinetic properties of each reaction have an important role in controlling the reaction mechanisms and the values can be found in the literature sources [17, 26-28]. Coal particles' interaction with the fluid region is dealt with through the Lagrangian multi-phase model. Coal particle properties are defined and an injector is set up in order to control the particle injection into the furnace. The injector is set for injecting coal particles continuously into the reactor. The reaction mechanisms and kinetic parameters used for the gasification reactions are shown in Table 1.

The coal particles used in the simulations are bituminous coal samples PSOC 1451. The properties, such as its proximate and ultimate analyses can be seen in Ref. [8, 20, 29-31]. The numerical simulations were conducted under quiescent gas conditions in the gasifier [21, 22, 32]. It was set by turning off the hot air flows a few seconds prior to the particle injection [31-33]. This treatment supports the creation of a homogeneous furnace gas temperature at around 1400K.

3 Investigation of gasification behaviour at various environments

The addition of H_2O [34] is designed to form a better syngas product [12], and the addition of CO_2 is aimed to investigate the potency of the CO_2 utilisation in the gasification [35-37]. It is a response to the environmental issue of coal utilisation through the gasification process, and identify the effect of *Boudouard* reactions ($C + CO_2 \rightarrow 2CO$) on the gasification processes

[13, 38]. It is also possible to identify the influences on the gaseous products when both gases are added and combined into the reactor at a certain fraction. The operation and boundary conditions were set the same. A coal particle with a diameter of $75\mu\text{m}$ was injected into the reactor every 50ms until a steady-state condition was reached. The injection process took about 20 seconds.

3.1 Effect of steam (H_2O)

Varying steam (H_2O) concentrations are considered to investigate its effects on coal gasification [39]. Three cases with the mole fraction of H_2O being 20%, 40%, and 60% (with 20% of O_2 and the rest was N_2) were simulated to present steam additions in the reactor, respectively. The coal gasification under air (20% O_2 & 80% N_2) condition was presented as a reference case. The compared results of the numerical simulations are shown in Figure 3 and 4.

Figure 3 initially demonstrates the profiles of the particle temperature and the char fraction during the gasification process under different gasification environments. It can be clearly seen that the particle temperature is higher under the lower H_2O mole fraction conditions. It is because the more steam requires further heat, and therefore the particle temperature slightly drops. However, the char fraction profiles were almost similar for every condition. This indicates that the steam added into the gasification reactor potentially drops the coal temperature but it has no significant effect on the char reactions.

Meanwhile, the results of CO & H_2 ; and CH_4 & CO_2 products under various H_2O concentration conditions are illustrated in Figure 4(a) and (b), respectively. Figure 4(a) shows that supplying steam (H_2O) into the reactor potentially increases the gaseous H_2 production but it has no significant effect on the CO formation. However, compared with gasification under air environment, the CO formation is much lower under the environment existing H_2O . It is possible because more H_2O reacts with CO to form CO_2 (see Table 1), and therefore CO_2

slightly increases. However, this indicates that the addition of steam promotes H_2 production in the gasification products, but it decreases the CO productions.

Figure 4(b) reports the production of CH_4 and CO_2 under various mole fractions of H_2O compared with air as a reference case. It is shown that, there is more CH_4 produced during the gasification process when the concentration of H_2O increases while the formation of CO_2 shows little difference under different environments. It is because of the increase of H_2 , and it also supports the formation of CH_4 (see the mechanisms in Table 1). However, it indicates that the addition of H_2O into the gasifier potentially increases the CH_4 production.

3.2 Effect of CO_2

In order to identify the potency of CO_2 utilisation in the gasification process [36-37], a simulation through coal particle reactions is performed. As an initial performance, a single coal particle injected and simulated under the two different reactor's environments: air (20% O_2 & 80% N_2) and CO_2 addition (20% O_2 & 60% N_2 & 20% CO_2). The performance is investigated with the production of CO and H_2 under these two conditions, and the results are shown in Figure 5.

It is found that the maximum value of CO and H_2 with the addition of CO_2 in the environment of the reactor is higher than that with air. But after approximately 50ms, the mole fraction of H_2 under air environment is slightly higher than that under the addition of CO_2 conditions. However, it is still an indication of the potency higher H_2 and CO formation with the addition of CO_2 . Therefore, in order to produce more evidence and results, further investigation was performed with continuous coal injections. For this, three additional cases were developed with CO_2 concentration varying at 20%, 40%, and 60% (with 20% O_2 and the rest is N_2), respectively. Here, the results under the air condition were shown as a reference case as well. The compared results of the particle temperature and char mass fraction are reported in Figure 6. As seen in the figure, the temperature of the coal particles,

with the addition of CO_2 are slightly lower than that at the condition with air, but there is almost no difference in the char percentages. The lower temperature at the higher CO_2 addition identifies that the reactions with CO_2 are endothermic (requiring heat) [26] and therefore causes the decrease of temperatures. However, this simulation clarifies that the addition of CO_2 potentially reduces the temperature and has no significant effect on the char reaction.

The formation of gaseous species of CO , H_2 and CH_4 under various CO_2 mole fraction conditions is also presented in Figure 7. Figure 7(a) shows that the addition of CO_2 in the reactor has the power to increase the quality of syngas products. This shows that the products of CO and H_2 in the environment with the addition of CO_2 are higher than those in the air environment. It also identifies that the reactions of CO_2 in the mechanisms (see Table 1) produce CO and/or H_2 , therefore both gases increase. This further demonstrates the merits of adding CO_2 in the gasification process.

Figure 7(b) shows the impact of adding CO_2 on CH_4 . It shows that CH_4 increases with the addition of CO_2 in the reactor, and it can be caused by the increase of H_2 during the reactions (as per the mechanisms shown in Table 1). This is, therefore, also another good indication of the gasification process, since all the syngas products show an increase through the addition of CO_2 to the reactants.

3.3 Combining H_2O and CO_2 with excess oxygen

Numerical simulations of coal gasification with a mixture of H_2O and CO_2 into the reactor has been conducted to investigate the effect of combining H_2O and CO_2 on the syngas production. While running the simulations, the reactor is set with the gaseous environment consisting of CO_2 and H_2O at a certain ratio, and 20% of O_2 is set as a constant for each case to allow the coal oxidation reactions to take place. The simulations performed in the ratio of

CO₂ and H₂O are 20/60, 30/50, 40/40, 50/30 and 60/20, respectively, and the gas products of the reaction are compared.

Figure 8 shows that the increase in the ratio of CO₂/H₂O potentially increases the particle temperature, and the char fraction looks similar for each case. This indicates that the increase of CO₂ has a greater effect on the increase in the temperature rather than H₂O, while the changes in both CO₂ and H₂O have no significant effect on the char reactions. However, Figure 9(a) shows that the increasing ratio of CO₂ and H₂O produces more CO, but less H₂ products. This therefore indicates that the addition of CO₂ has a greater effect on the CO formation, while the addition of H₂O has a greater effect on the H₂ formation. Meanwhile, Figure 9(b) shows that the increase in the ratio of CO₂ and H₂O potentially produces less CH₄. This, thus, further indicates that the CH₄ formation is more influenced by H₂O rather than CO₂.

3.4 Combining H₂O and CO₂ without oxygen

The condition when CO₂ and H₂O were combined with the absence of oxygen potentially occurred in the gasification process. Particularly in the UCG (Underground Coal Gasification) application, the condition occurred mostly in the reduction zone. Therefore, it is important to investigate the behaviour affected by this condition. To present the investigation, the simulations are performed similarly as in the previous section, but with the absence of oxygen fractions. The reactor is filled with CO₂ and H₂O at a certain ratio; 20/80, 40/60, 50/50, 60/40 and 80/20, respectively.

Figure 10 shows that the increase in the CO₂ and H₂O ratio results in higher particle temperatures. It indicates that the coal reactions in the environment consisting more H₂O produces more heat than in the environment consisting more CO₂. However, the maximum particle temperature is very low compared to that in the presence of oxygen (see Figure 8.). It therefore indicates the coal oxidation reaction does not occur. The affirmation is verified by

the trend of the char fraction profile, which decreases but very slowly or almost insignificantly. The almost similar trend of char reaction is found for each fraction level.

While comparing the results of H_2 , CO and CH_4 , reported in Figure 11, Figure 11(a) shows that the increase in the CO_2 and H_2O ratio promotes the production of CO but decreases H_2 . However, the CO formation in the absence of oxygen is slower than that in the presence of oxygen (see Figure 9 for comparison). On the other hand, H_2 production in this figure keeps increasing, with the level of concentration being also higher with oxygen inclusion (see Figure 9). This indicates that this condition is preferable for the H_2 formation rather than CO.

Further, Figure 11(b) illustrates the CH_4 formation under varying CO_2 and H_2O ratios, with the absence and existence of oxygen. The case with the absence of oxygen has already been described in the previous section and Figure 11(b) confirms it. It clears that CH_4 is more affected by H_2O than CO_2 and the increase in CO_2 and H_2O ratios causes the decrease in CH_4 . With regard to the existence of oxygen, Figure 11(b) shows that CH_4 production is higher and more stable in the condition with oxygen, but the trend of CH_4 formation in the condition without oxygen is consistent with an increase. However, the simulation results show that CH_4 formation occurred in both conditions, with or without oxygen.

4 Effect of coal particles' size and reactor's temperature

4.1 Coal particles' diameters

The gasification simulations are conducted with three different coal sizes ($60\mu m$, $75\mu m$ and $100\mu m$) under the air environment. The coal particles were injected every 50ms within 20s into the reactor and the temperature of air was 1400K. A comparison of the results of syngas production can be seen in Figure 12.

Figure 12(a) reports the contour plots of the molar concentration of H_2 with different size of coal particles. It is shown that the bigger coal particle has a greater area of gas distribution in

the contour plot, but the level of concentration seems to be lower. This is because the bigger coal particle experiences a larger imbalance between the gradational and aerodynamic drag forces which causes the free-fall particle to move faster inside the reactor. The gas products then fill the space along the particle displacement and finally develop a greater area with lower concentration. It is possible that the H_2 product further reacted with oxygen or char to produce CH_4 and H_2O according to the reaction mechanisms as shown in Table 1, and therefore the concentration seems weaker along the gas stream (axis direction). Further, the smaller particles accumulated the production of H_2 in a smaller area of the reactor and, therefore, a higher concentration level is observed.

Other species of syngas products, such as CO and CO_2 , can also be presented to identify the effect of particle size as shown in Figure 12(b) and (c), respectively. These figures show that the changing trends of CO and CO_2 are similar to that of H_2 . The bigger particle size covers a greater area in the reactor but with a lower level of gas concentration. For CO, as shown in Figure 12(b), the concentration also seems to be weaker along the particle flow, and it is possible that CO has further reacted with oxygen to produce CO_2 as defined in Table 1. Having the same trend as CO and H_2 , the distribution area of CO_2 concentration looks greater in the reactor, as shown in Figure 12(c). This indicates the production of CO_2 is much more than other gases in this simulation. It is understandable since, at this stage, according to the gasification mechanisms defined in Table 1, the simulation has excess oxygen or it has been undertaken at lean combustion conditions.

The figures of contour plots present the mole gas concentration over the volume of the reactor. It is helpful to clarify the gas product distribution of each coal particle and gasification inside the reactor. However, as a comparison value of gas concentration produced over the area of generation by each particle size, see Figure 13.

Figure 13(a) and (b) show the comparison of the mole fraction of gaseous products CO & H₂, and CH₄ & CO₂ with different sizes of coal particles, respectively. Figure 13(a) shows that the coal particles in large sizes produce more H₂ but the less CO after reaching steady state condition. The greater H₂ production can be explained by noting that the increasing particle diameter causes an increase in the reactants' mass (i.e. char fraction and coal volatile), and this leads to an increase in mass products as well. In addition, H₂ is produced dominantly from homogeneous reactions (see Table 1), which is not affected by particle size. In contrast, CO is mostly produced from heterogeneous reactions, and therefore the effect of particle size is significant.

Figure 13(b) further shows that the larger coal particle size results in a slightly higher level of CO₂, and lower CH₄ in the products. The increase in the reactant's mass increases the product of reactions, as in CO₂. Although the CO₂ is produced dominantly from heterogeneous reactions, the effect of additional coal mass gives greater significance to the products' formation. Meanwhile, CH₄ behaviour indicates a similarity with the CO. This is because the CH₄ formation (as shown in Table 1) is obtained from the heterogeneous reactions, which indicates that they are affected by the particle size. The smaller particle size potentially produces more products.

4.2 Performance under various temperatures

The influence of temperature on the gasification reactions was studied to identify the performance behaviour. For this purpose, the three temperature conditions (1000 K, 1200 K and 1400 K) of the reactor are set for gasification simulations. These variation in number refers to the temperature variation study according to *Bhutto et al.* [12]. For the operation conditions, the coal particles with a diameter of 75 μm were injected into the reactor and air was considered as a gasification agent in this case. The simulations were performed for 20s.

It can be clearly seen in Figure 14 that the formation of H_2 in the gasification process is affected by the temperature of the reactor. First, the gasification process under higher temperature conditions has an earlier H_2 formation. As evidence, this can be seen at the temperature of 1400K, the outer contour of H_2 cloud is much closer to the inlet of coal injection while it is farther away from the inlet region at lower gasification temperatures. Moreover, compared with the low temperature cases, the molar concentration of H_2 is greater at higher temperature conditions. These indicate that the higher temperature of reactor obtains a higher production of H_2 .

For further identification, the molar concentration of CO and CO_2 inside the reactor can be seen in Figure 14(b) and (c), respectively. Figure 14(b) shows the distribution area of CO and CO_2 in the contour plot of the reactor. The formation behaviour of CO shown in Figure 14(b) is similar to that of H_2 shown in Figure 14(a). The higher reactor temperature has a greater plot area, which indicates the greater CO production obtained in the reactor at 1400K. Meanwhile, CO_2 production is greater at the higher temperature of the reactor as shown in Figure 14(c). These results clarify that the gas production obtained was greater at the higher temperature of the reactor.

Those results are described qualitatively and they need to be compared in values quantitatively in order to have a better comparison, which are shown in Figure 15. It represents the molar fraction of the gaseous products of H_2 , CO, CO_2 and CH_4 during the gasification process.

Figure 15(a) shows the comparison in earlier contour plot results, and this confirms that the higher temperature results in more H_2 and CO production. After about 5s coal injection, the trend of H_2 and CO are stable, and still consistent that at higher temperature more H_2 and CO are produced. Other results are CO_2 and CH_4 , as shown in Figure 15(b). This figure also confirms that at a higher temperature, greater CH_4 and CO_2 production is obtained.

5 The behaviour of particles' temperature and CH₄ formation

The temperature of coal particles is a parameter that can also be used to identify the reaction stages of coal gasification [40], and it has an important role to form the anticipated products [12]. Therefore, it becomes a parameter of this study and, through the coal particle model, the coal's temperature behaviour can be identified during the reactions. On the other hand, the formation process of CO₂, CO, and H₂ during the gasification reactions along the reactor has been described in the previous study [8]. To complement the investigation, this study describes the behaviour of CH₄ formation during the reactions.

During the gasification simulation, coal particles were continuously injected into the reactor with 500 times much more than the simulation cases presented in Sections 3 and 4, with the air flow under the quiescent gas condition. The oxidation reactions are propagated downstream because of the presence of air, and the reduction reactions occur simultaneously at the back the oxidation. The coal particles' temperature inside the reactor after several occurrences of the reaction can be seen in Figure 16. The figures are shown in a sequence of time in order to identify the process over that period. It can be seen the coal particles were burned and, because of the gravity, they flow along the axis. The peak particle's temperature occurred on the spot where the coal contacts with oxygen, and over the time it decreases. Meanwhile, the coal particles were continuously injected, and because of the absence of oxygen, it was not burnt. This identification matches the coal particle temperature's behaviour that was described in Section 3.4 where it showed that the particle's temperature did not increase at the condition without oxygen (see Figure 10).

The coal particles keep injected at the spot near the inlet as can be seen in Figure 17. This figure also used to identify the CH₄ formation inside the reactor, during the reactions. Figure 17 shows the behaviour of CH₄ formation based on the result of simulation. After 50s of the coal injection, the spot of CH₄ formation is dominated in the coal injection's area. This

behaviour is similar with the contour plot of H_2 formation as in our previous study (see in Ref. [8]), but the area is smaller. This also indicates the correlation between the CH_4 and H_2 formation, which is relevant to the reaction mechanism defined in Table 1. The results also show that, if the CH_4 decreases in the downstream area, this was possibly caused by its reaction and distribution through the reactor.

The gas production behaviour, as explained earlier, describes the thermochemical process of the chemical reaction mechanisms as defined for coal gasification. The simulation results have clarified the syngas production in each stage and correlation among the species in the reaction has also been identified.

6 Conclusion

Numerical simulations through the model of coal particle performance have been carried out for the investigation of the thermochemical behaviour of gasification reactions. This study focused on improving the syngas quality with the addition of steam (H_2O) and CO_2 . The results of simulation showed that the addition of H_2O on the gasification reactions increased the H_2 and CH_4 productions. Meanwhile, the CO_2 utilisation for the process of gasification increased the production of CO , H_2 and CH_4 . However, both gaseous additions into the gasification reactions decreased the temperature of coal.

Other simulation performance was conducted with an aim to identify the effects of particle's size, and the results of simulation showed the particle size affected the gas performance, specifically on the heterogeneous reactions.

The variation of reactor's temperature was inclusive in the study to identify the effect on the syngas formation. The results showed that more gas products obtained at the gasification process with the higher reactor's temperature.

Overall, these results indicated a good agreement with the other studies of coal gasification from several sources. Therefore, it potentially can be used as a guideline for obtaining better

quality syngas production. Additionally, by using the performance of coal particle model, the complex processes during gasification reactions were identified, and the study could also be further developed for obtaining a robust coal gasification technology.

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Table 1. The kinetic parameter values used in gasification reactions

Mechanisms	Reaction no	Kinetic parameters			Ref.
		A (unit vary)	E_a (j/kmol)	β	
Raw coal $\rightarrow$ Coal volatile + Char	R1	3.12E+05	7.40E+07	0	[41]
C + O ₂ $\rightarrow$ CO ₂	R2	0.002	7.90E+07	0	[41]
C + 0.5O ₂ $\rightarrow$ CO	R3	85500	1.40E+08	0.84	[42]
C + CO ₂ $\rightarrow$ 2CO	R4	4.4	1.62E+08	1	[41, 43]
C + H ₂ O $\rightarrow$ CO + H ₂	R5	1.33	1.47E+08	1	[41, 43, 44]
C + 2H ₂ $\rightarrow$ CH ₄	R6	1000	1.13E+08	0	[45]
Coal Volatile + O ₂ $\rightarrow$ CO ₂ + H ₂ O + N ₂	R7	2.12E+11	2.03E+08	0	[41]
CO + 0.5O ₂ $\rightarrow$ CO ₂	R8	1.30E+11	1.26E+08	0	[41, 44]
H ₂ + 0.5O ₂ $\rightarrow$ H ₂ O	R9	1.50E+13	2.85E+07	0	[46]
CO + H ₂ O $\rightarrow$ CO ₂ + H ₂	R10	4.20E+07	1.38E+08	0	[45]
CH ₄ + H ₂ O $\rightarrow$ CO + 3H ₂	R11	4.40E+11	1.68E+08	0	[42]
CH ₄ + 0.5O ₂ $\rightarrow$ CO + 2H ₂	R12	3.00E+08	1.26E+08	-1	[42]
CH ₄ + CO ₂ $\rightarrow$ 2CO + 2H ₂	R13	4.60E+11	3.12E+08	0.3	[47]

Figure 1. Process illustration of coal particle gasification reactions

Figure 2. The furnace illustration (a) Furnace cylindrical shape (b) Axisymmetric model grid

Figure 3. The particle temperature and char profile in H₂O environment

Figure 4. Gas production under various H₂O conditions: (a) H₂ & CO, and (b) CH₄ & CO₂

Figure 5. Particle temperatures and char mass fraction comparisons

Figure 6. Particle temperature and char mass fraction in CO₂ variations

Figure 7. Gas products comparisons in CO₂ variation (a) CO & H₂, and (b) CH₄

Figure 8. Particle temperature and char mass fraction in the $\text{CO}_2/\text{H}_2\text{O}$ variations

Figure 9. The gas productions in some CO₂ and H₂O ratios, for (a) CO& H₂, and (b) CH₄

Figure 10. Particle temperatures and char fractions' comparison in $\text{CO}_2/\text{H}_2\text{O}$ ratio variations

Figure 11. Gas products comparisons in the CO₂/H₂O ratio variations for (a) H₂ & CO, and (b) CH₄

Figure 12. Molar concentration in a variation of coal particle diameters after 20s, for gas (a)

H_2 (b) CO and (c) CO_2

Figure 13. Mass average mole fraction results for (a) CO & H₂, and (b) CO₂ & CH₄

Figure 14. Molar concentration of gas products in various temperatures after 20s, for (a) H₂
(b) CO, and (c) CO₂

Figure 15. The gas products at temperature variations, for (a) H₂ & CO, and (b) CH₄ & CO₂

Figure 16. Contour plot of reactor temperature

Figure 17. Contour plot of CH₄ inside the reactor