

Numerical Simulation of Pressurized Spouted Fluidized Bed for Coal Semi-Gasification^{*}

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Abstract: Numerical simulation study is conducted for a pressurized spouted-fluidized bed coal carbonizer, in which hydrodynamics of pressurized spouted-fluidized bed, chemical reactions and energy balance are taken into account. The effect of operating conditions such as bed pressure, air and steam mass flow ratio, temperature on product compositions in the bed is investigated. According to the calculated results, bed pressure and bed temperature have the key effects on coal semi-gasification.

Key words: pressurized spouted-fluidized bed, coal gasification, numerical simulation

The second generation advanced pressurized fluidized bed combustion (APFBC) uses a carbonizer for partially gasifying coal to generate low-Btu fuel gas for the APFB cycle system. The low-Btu fuel gas blends with the off-gas from PFB boiler and combusts with the remaining oxygen in the off-gas, which results in the mixing gas to a higher temperature (above 1100? °C) at the inlet of the gas turbine. As a result, significantly improvement in APFBC-CC efficiency will be achieved as more efficient, high temperature gas turbines are employed. It is obvious that the optimization of the design and operation of the carbonizer is vital to the APFBC-CC system. Provided that the reaction process in the carbonizer is mainly coal gasification and there has been extensive experience of research and development on common coal gasification. The coal gasification is different, which focusing on char residue reactivity, low capital cost and low environmental emission rather than concerning with high char conversion in common gasification. Therefore, it is still lack of reliable data specially for carbonizer design and operation. Recently, the British adopted a spouted bed carbonizer in power generating system, which combined semi-gasification and combustion, called air blown gasification cycle (former topping cycle process)^[1]. The spouted-fluidized bed carbonizer is considered to combine properties of fluidized and entrained bed since the annulus is a fluidized bed while the cyclic motion of particles through the spout and fountain ensures good mixing. Many experiments have been performed to find

a better way for the spouted-fluidized bed design and control, yet its unknown fluid mechanic characteristics lead to difficult to optimization.

Experimental investigations have been performed on coal gasification in almost all kinds of carbonizer types^[2-4]. Models on fixed, fluidized, jet fluidized and spouted bed have also been proposed by many researchers. In the development of spouted fluidized bed carbonizer, because of difficulty of measurements, numerical modeling and simulation are useful for gaining an insight into the influence of design parameters, coal properties and operating parameters on the carbonizer performance.

Many models on flow in spouted or spouted-fluidized bed have been proposed, which can be classified into two groups. The first group is using the mass, momentum and energy equations to describe the turbulent flow^[5,6]. After several decades of developing, the progress is obvious and many phenomena can be interpreted by these models. Nevertheless, their solutions are based on one or more assumptions, which seems a bit far from reality. Along with the deeper and deeper insight into the bed hydrodynamics and the development of more powerful computers, their future is promised. Another group is empirical, which divides the bed into several zones (mostly two zones, spout and annulus) according to its flow pattern^[7-13]. Empirical correlations are used to simulate characteristics in different zones. The accuracy of these models depends on their experimental data. But it is unsuitable for predicting even a slightly different types

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of bed due to its superficial characteristics.

As for the chemical reactions, two kinds of models are also used. One is based on chemical equilibrium theory, considering infinite reaction rate and all reactions reaching their equilibrium. So equilibrium coefficient of each reaction can be used to calculate all compositions in the gas. Another is based on kinetic models considering the reaction kinetics^[2, 11]. If the kinetic data of reactions is known, the rate of each reaction can be calculated.

In this work, a numeric model is supposed combined flow and chemical reactions to simulate a pressurized spouted-fluidized bed carbonizer. All the units for pressure are kPa.

1 Modeling Flow in Spouted Fluidized Bed

According to gas-solid flow pattern, the bed is empirically divided into two zones, the spout zone from the bottom to the fountain and the freeboard zone above the spout part. Each zone consists of several parts, shown in Fig.1. In the center of the bed, there is a spout part due to high velocity of gas inlet. Around the spout part is the annulus part which is a dense phase field. Gas flows from the spout at a little high speed in the freeboard zone and forms a fast part in the center. Around the fast part is the slow part where gas flows slower. Particles flow up to a certain height and then fall down or move sideward to the slow part and back to the annulus part of spout zone.

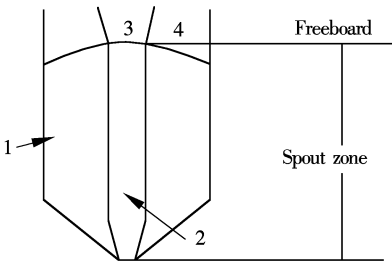


Fig.1 Spouted fluidized bed

1—annulus; 2—spout; 3—fast flow part; 4—slow flow part

1.1 Spout zone

According to the experiment, the fountain diameter varies with bed height within a certain distance. Above that distance, the spout diameter changes little. The diameter of spout in its developing stage can be expressed as

$$\frac{d_j - d_{or}}{d_{or}} = 2.14 \left(\frac{\rho_g u_{or}^2}{(1 - \epsilon) \rho_s d_p g} \right)^{-0.25} \cdot \left(\frac{h}{H_p} \right)^{-0.49} \left(\frac{P}{P_0} \right)^{2.35} \quad (1)$$

where d_{or} is nozzle diameter; d_j is spout diameter; d_p is particle diameter; ρ_g , ρ_s are density of gas and solid; h is bed height; H_p is maximum bed height; u_{or} is gas inlet velocity at nozzle; P is the bed pressure; P_0 is atmosphere pressure. The diameter above the distance is developed by Horio, et al^[1].

$$d_j = 0.78 d_{or} \left(\frac{f_j F_{ij}}{\sqrt{k} \tan \alpha} \right)^{0.3} \left(\frac{d_{or}}{D_c} \right)$$

where α is the bottom geometry angle; D_c is the bed diameter; $f_j \approx 0.02$; $F_{ij} = \rho_g u_{or}^2 / ((1 - \epsilon_{mf}) \rho_p d_p g)$; $k = (1 - \sin \alpha) / (1 + \sin \alpha)$.

The correlation of net gas exchange between spout and annulus was given by modified Lefry-Davidson equation^[1]

$$\frac{U_{th}}{U_{aj,hj}} = \left(\sin \frac{\pi h}{2h_m} \right)^{0.5} \quad (2)$$

where U_{th} is net gas volume flowing from spout to annulus; $U_{aj,hj}$ is gas velocity at the out let of annulus; h_m is maximum bed height; $U_{aj,hj} = CU_{mf}$, U_{mf} is minimum fluidized spouted velocity, C is a fitting parameter varying from 0 to 5. U_{mf} can be calculated by^[14]

$$\frac{U_{mf} \rho_g d_p}{\mu} + 33.7 = \left(33.7 \times 33.7 + 0.408 \frac{d_p \rho_g g (\rho_p - \rho_g) g}{\mu^2} \right)^{1/2} \quad (3)$$

Between the spout and annulus, there exists gas passing through the interface, i.e. gas in the spout flows to annulus through interface and the same amount of gas is entrained to spout from annulus. The exchange velocity equation is given by^[1]

$$\left. \begin{aligned} U_{ex} &= KU_a \\ K &= \tan \beta \end{aligned} \right\} \quad (4)$$

where U_{ex} is gas exchange between spout and annulus; U_a is gas velocity in annulus; β is the spout angle.

In the spout, both particles spouted from nozzle and entrained from annulus flow with stream due to high gas velocity till they reach the freeboard zone. The slip velocity U_t between particles and gas can be found in literature.

The mass of entrained particles from annulus to spout W_s was developed by Patose and Caram^[1]:

$$\frac{W_s}{W_{s,hm}} = \frac{h}{h_m} \left(2 - \frac{h}{h_m} \right) \quad (5)$$

where

$$W_{s,hm} = A_m \rho_p (gH)^{1/2} \left((1 - \epsilon_{sh}) \left(\frac{\rho_p - \rho_g}{\rho_p} \right) C_o (\epsilon_{sh} - \epsilon_{mf}) \right)^{1/2} \quad (6)$$

$$\epsilon_{sh} = \frac{(h_m/H) + 0.937 \epsilon_{mf} C_o}{(h_m/H) + 0.937 C_o}$$

The value of C_o is estimated as

$$C_o = \begin{cases} 0.7 & 0.8 < h_m/H \\ 0.65 & 0.5 < h_m/H \leq 0.8 \\ 0.55 & h_m/H \leq 0.5 \end{cases}$$

The particle hold-up ϵ_s in the fountain can be calculated as

$$\epsilon_s = \frac{W_j}{A_j V_{fj} \rho_s} \quad (7)$$

So gas velocity at any height in spout U_j can be calculated by

$$U_j = \frac{Q_j}{A_j (1 - \epsilon_s)} \quad (8)$$

where W_j , Q_j are the total solid flow rate and gas flow rate, respectively. In the present model, a constant voidage, ϵ_{mf} , is employed in the annulus part. A_j is the cross area of spout.

1.2 Freeboard zone

Since the velocity in freeboard zone is slow, particles entrained from slow part to fast part are ignored. The mass of gas M_h entrained from slow part to fast part is calculated by

$$M_h = 0.32 \frac{H_f}{d} \quad (9)$$

where H_f is the height in freeboard.

$$d \approx 2 \sqrt{4(Q_j + m_h/\rho_g)/U_{gl}} \quad (10)$$

From energy balance:

$$\frac{1}{2} m_g U_g^2 + \frac{1}{2} M_h U_a^2 + \frac{1}{2} m_s U_s^2 = m_s g H + \frac{1}{2} (m_g + M_h) U_{gl}^2 \quad (11)$$

$$U_{gl} \approx \frac{Q_j + Q_a}{A_j} \quad (12)$$

where $Q_j + Q_a$ is the total gas flow rate in freeboard. Using Eq. (11), the terminal divergence height H can be calculated. The momentum balance based on different height can be described as follows, neglecting the wall effect and solid collision.

$$\rho_p \left(\frac{\pi d_p^3}{6} \right) \frac{dV_j}{dt} = (\rho_p - \rho_g) \left(\frac{\pi d_p^3}{6} \right) g + C_d \left(\frac{\pi d_p^2}{4} \right) \frac{\rho_g (U_{fj} - V_j)^2}{2} \quad (13)$$

where $C_d = \frac{24}{R_e} (1 + 0.125 R_e^{0.72})$

$$R_e = \frac{d_p (U_{fj} - V_j) \rho_g}{\mu}$$

From the above differential equations, the particle velocity can be solved in fast flow part. Therefore the particle hold-up ϵ_{fs} can be computed as

$$\epsilon_{fs} = \frac{W_j}{A_j V_{fj} \rho_p}$$

$$U_{fj} = \frac{Q_{fj}}{A_{fj} (1 - \epsilon_{fs})}$$

where A_{fj} is the cross-area of fast part of freeboard. Using Kunii and Levenspiel model^[14], the voidage of slow flow part can be expressed as

$$\epsilon_{fa} = \epsilon_{mf} \exp(-ah) \quad (14)$$

where a is the decaying parameter.

2 Particle Mass Balance

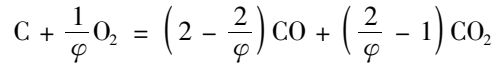
In a spouted fluidized bed, the particle size distribution can be taken as uniform in the annulus part. In the spout, the most of the particles are entrained from annulus. So it is acceptable to assume that the particle size distribution is uniform.

Provided that the particle size distribution of mass of inlet particle, sediment flying ash and particle in bed are $P_0(d_p)$ and M_0 , $P_1(d_p)$ and M_1 , $P_2(d_p)$ and M_2 , $P_b(d_p)$ and M_b . Using Kunii and Levenspiel model^[14], the relationship can be expressed.

3 Reaction Kinetics

3.1 Oxidation

Oxidation occurs in fountain and at the bottom of annulus which provides the heat for coal gasification. It can be expressed as^[15]



where φ is the fitting parameter and can be estimated as

$$z = 2?500 \exp(-6?249/T), \varphi = 1.0 \text{ if } d_p > 1 \times 10^{-3} \text{ m}$$

$$\varphi = (2z + 2)/(z + 2) \text{ if } d_p \leq 5 \times 10^{-5} \text{ m}$$

$$\varphi = ((2z + 2) - z(d_p - 5 \times 10^{-5})/9.5 \times 10^{-4})$$

if $5 \times 10^{-5} \text{ m} < d_p \leq 1 \times 10^{-3} \text{ m}$

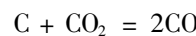
The reaction rate is^[15]

$$r_1 = P_{O_2} S / (1/k_{sl} + 1/K_{dl}) \quad (15)$$

where $k_{sl} = 8.6 \times 10^2 \exp(-18?000/T_p)$.

3.2 Carbon dioxide gasification

It is one of main reactions in coal gasification process.



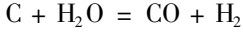
The reaction rate is^[15]

$$r_2 = P_{CO_2} S / (1/k_{s2} + 1/K_{d2}) \quad (16)$$

where $k_{s2} = 1.35 \times 10^{-1} \exp(-16?300/T)$.

3.3 Steam gasification

Another main reaction in coal gasification process is the steam gasification.



The reaction rate is^[15]

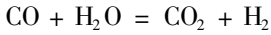
$$r_3 = P_{\text{H}_2\text{O}} S / (1/k_{\text{s3}} + 1/K_{\text{d3}}) \quad (17)$$

where $k_{\text{s3}} = 1.92 \exp(-177680/T)$, $T = \frac{T_{\text{g}} + T_{\text{p}}}{2}$.

In (15) – (17), T_{p} is the temperature at the particle surfac; T_{g} is the gas temperature; S is the particle surface area.

3.4 Steam gas shift reaction

This reaction changes the volume of CO and H_2 .

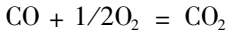


It is reported that the reaction is affected by certain metal elements in coal particles. In the model, such affection is ignored. And Eq.(18) is employed^[1]:

$$r_4 = \frac{k}{RT_{\text{g}}^2} \left(P_{\text{CO}} P_{\text{H}_2\text{O}} - \frac{P_{\text{CO}_2} P_{\text{H}_2}}{K_{\text{eq}}} \right) \quad (18)$$

where $k = 27780 \exp(-17510.7/RT_{\text{g}})$; $K_{\text{eq}} = 0.265 \cdot \exp(397565/T_{\text{g}})$.

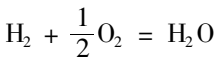
3.5 Carbon monoxide combustion



The mechanics of the reaction is unknown yet. In the article, model developed by Hotel, et al. is used.

$$r_5 = 3 \times 10^{10} \exp(-167000/RT_{\text{g}}) f_{\text{CO}} \times (17.5 f_{\text{O}_2} / (1 + 24.7 f_{\text{O}_2})) f_{\text{H}_2\text{O}}^{1/2} \quad (19)$$

3.6 Hydrogen combustion



The reaction occurs rapidly, its rate is^[16]

$$r_6 = 2 \times 10^{-11} \exp(-747500/RT_{\text{g}}) \quad (20)$$

4 Coal Devolatilisation Modeling

In a spouted fluidized bed, the temperature can reach as high as 1700°C. It can be assumed that the volatile composition consists of H_2 , CO_2 , CO and H_2O . Assuming that all H and O elements in coal particles are releasing, the volatile compositions can be estimated based on element balance.

The escaping rate of each composition can be calculated as^[17]

$$\frac{dV_i}{dt} = k_i (V_i^* - V_i) \quad (21)$$

where V_i^* means the maximum volume of volatile composition i ; $k_i = k_{oi} \exp(-E_i/RT_{\text{p}})$; k_{oi} and E_i are listed in Tab.1.

Tab.1 Dynamics of CO , H_2 , CO_2 , H_2O ^[17]

Product gas	K_o/s^{-1}	$E/(kJ \cdot mol^{-1})$
H_2	3.6×10^3	106.3
CO_2	33	40.6
CO(stage 1)	7×10^3	86.3
CO(stage 2)	1.1×10^5	144.9
H_2O	27	41.5

5 Energy Balance

5.1 Spout zone

In the spout zone, although there is some temperature difference between particles and gas in the lower part of the annulus and spout due to combustion of coal in the spout. Such a difference is ignored in the model. The temperature is taken as uniform due to gas intensive blending in the spout and mass exchanging between two parts and fluidizing gas agitation in annulus.

Now, the energy taken into spout zone is

$$m_0 C_{\text{pC}} t_1 + C_{\text{pa}} m_{\text{a}} t_2 + C_{\text{pst}} m_{\text{st}} t_3 + m_0 Q_{\text{dw}}^y \quad (22)$$

Terms of expression (22) represent the heat of coal bringing in, heat of air bringing in, heat of steam bringing in and chemical energy of coal.

The energy taken out from spout zone is

$$m_1 C_{\text{pC}} t' + m_1' C_{\text{pC}} t_1' + \sum_{i=1}^5 C_{\text{pi}}' m_{\text{gi}} t_{\text{g}} + m_{\text{CO}} q_{\text{CO}} + m_{\text{H}_2} q_{\text{H}_2} + \Delta Q - m_1'' C_{\text{pC}} t'' + m_1' q_{\text{C}} - m_1'' q_{\text{C}} \quad (23)$$

where m_1 is the exit mass of coal; m_1' is the mass transferred from spout zone to freeboard; m_1'' is the mass returned from freeboard to spout zone; m_{gi} is the mass of gas composition i ; q_{CO} , q_{H_2} and q_{C} are the chemical energy of carbon monoxide, hydrogen and carbon, respectively; ΔQ is the heat loss.

In the model, the heat by particle entrained from spout zone to freeboard zone and the heat of particle returned to spout zone from freeboard are considered to be equal. In freeboard, the particle mass loss is little since chemical reaction is slow. So mass loss of particles is ignored in the model. So the energy transferred from spout zone to freeboard is the chemical energy loss of coal particles entrained by gas. Then expression (23) can be simplified as

$$m_1 C_{\text{pC}} t' + \sum_{i=1}^5 C_{\text{pi}}' m_{\text{gi}} t_{\text{g}} + m_{\text{CO}} q_{\text{CO}} +$$

$$m_{H_2} q_{H_2} + \Delta Q + m_2 q_c \quad (24)$$

Combined expressions (22) and (24), we can obtain

$$m_1 C_{pC} t' + \sum_{i=1}^5 C'_{pi} m_{gi} t_g + m_{CO} q_{CO} + m_{H_2} q_{H_2} + \Delta Q + m_2 q_c = m_0 C_{pC} t_1 + C_{pa} m_a t_2 + C_{pst} m_{st} t_3 + m_0 Q_{dw}^y \quad (25)$$

Let $t' = t_g$ and the temperature of spout zone can be calculated.

5.2 Freeboard zone

In the freeboard zone, combustion is over due to the lack of oxygen. The heat contained in the gas and particles supplies heat for gasification. So the temperature drops with the height increasing.

The freeboard is divided into slices along the bed height in the model. Assuming the temperature in each slice is uniform, the energy balance equation can be expressed as

$$\sum_{i=1}^5 C_{pi} m_{ij-\frac{1}{2}} t_{gj-\frac{1}{2}} + m_{Cj-\frac{1}{2}} C_{pC} t'_1 = \Delta m_{CO} q_{CO} + \Delta m_{H_2} q_{H_2} + \Delta Q' + \sum_{i=1}^5 C_{pi} m'_{ij} t'_{gj} \quad (26)$$

6 Results and Discussion

The analysis of coal is listed in Tab.2. The calculation condition and parameters are listed in Tab.3.

Tab.2 Coal properties

$w(C)/\%$	$w(H)/\%$	$w(O)/\%$	$w(N)/\%$	$w(S)/\%$	$w(FC)/\%$	$w(A)/\%$	$w(W)/\%$	$w(VM)/\%$
59.73	3.7	2.14	1.08	0.68	44.26	22.32	5.38	28.04

Tab.3 Calculation condition and parameters

Item	Value
Air inlet flow/($N \cdot m^3 \cdot h^{-1}$)	507
Steam inlet flow/($kg \cdot h^{-1}$)	105
Ratio of spouted gas to fluidized gas	7 : 3
Feed of coal/($kg \cdot h^{-1}$)	313
Fountain height/m	3.5
Diameter of nozzle/m	0.04
Diameter of bed/m	0.215
Pressure/Pa	5×10^5
$Q/(MJ \cdot kg^{-1})$	23.46
Density/($kg \cdot m^{-3}$)	1500
Mean particle size/mm	1.33

Fig.2 is the results of compositions varying with height in the spout. Along the height, the oxygen decreases quickly and steam is consumed at a certain rate. Before oxygen is exhausted, the carbon dioxide increases quickly, only a small fraction of hydrogen

and carbon monoxide exists in the stream. At the point of the oxygen exhausted, the carbon dioxide reaches its maximum. Above that height, the gasification is the dominant reaction. The hydrogen and carbon monoxide increase while carbon dioxide and steam decrease.

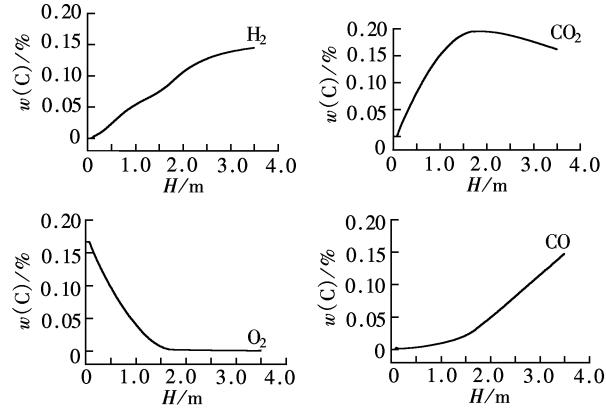


Fig.2 Gas composition in fountain

Fig.3 shows the result of compositions varying with height in the annulus. Near the distributor, oxygen drops sharply and the carbon dioxide increases fast while other compositions change little. This shows that the combustion is the main reaction within the area. Above that height, the oxygen is exhausted and temperature reaches a certain point. The coal gasification is the main reaction in annulus. The heat for the reactions is supplied by heat stored in particle and gas which is introduced from spout. Above a certain height, because of more volatile escaping and more gas introduced from spout, carbon monoxide and hydrogen increase obviously while carbon dioxide and steam decrease. As the height exceeds 2?m, the steam-gas shift reaction slows down and the temperature drops. Then the carbon monoxide increases and hydrogen-increasing rate decreases but its volume still increases.

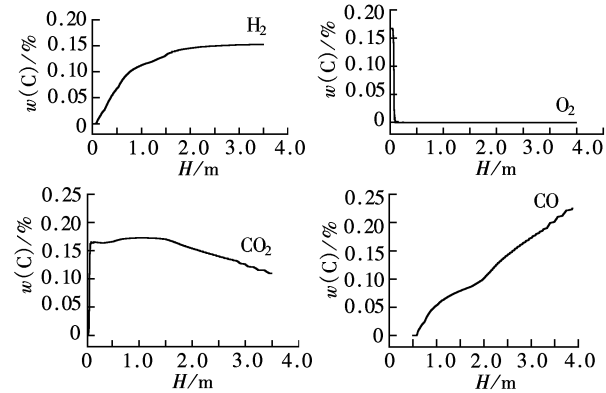


Fig.3 Gas composition in annulus

In the freeboard, the gasification process slows down since particle concentration decreases and

temperature drops. As shown in Fig.4, carbon monoxide increases, hydrogen changes little and carbon dioxide decreases. Composition profile in spout, annulus and freeboard is similar to the result of J. Bi^[1].

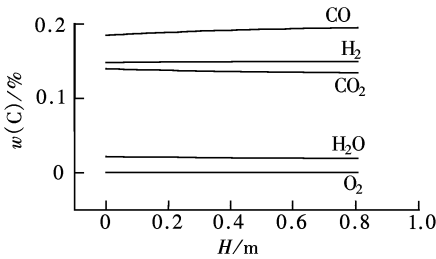


Fig.4 Gas composition in freeboard

Fig.5 shows the three main compositions and gas calorific capacity and bed temperature changing with bed pressure. While bed pressure increases, bed temperature drops and gas calorific capacity increases since carbon monoxide and hydrogen increase. So higher pressure is beneficial to coal conversion. This is quite different from J. Bi^[1]. According to their model, H₂ and CO decreased with the pressure increasing. It was the reason that the active carbon species inner surface became saturated with absorbed reactant gas molecules. But with the temperature above 1?100?°C, the diffusion dynamic factors are prevailing since chemical reaction rate is faster. Increasing bed pressure results in gas mass concentration, thus increasing gas diffusion rate. The gasification process is controlled by the kinetics within a certain pressure range. With the increase of pressure, reaction rate increases. More heat released from combustion converts to chemical energy which stored in gas. So the temperature drops down and gas capacity increases.

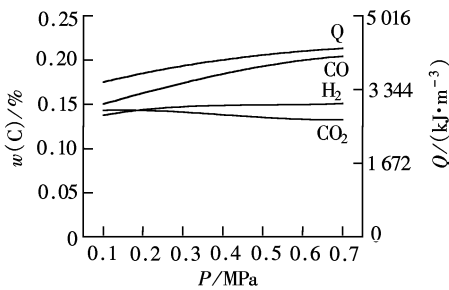


Fig.5 Pressure effect on CO,CO₂,H₂ and gas calorific capacity

Fig.6 is the effect of air/coal mass ratio β on compositions and gas calorific capacity. As the ratio increases, the combustion releases more heat and bed temperature rises. At the same time, part of the carbon monoxide is combusted and its percentage decreases. With the ratio increasing, the bed temperature drops

and reaction rate slows down. Also inertia gas N₂ is increasing. So the gas calorific value decreases. But the change is insignificant. This is similar to the experimental results by Y.J.Kim^[3] in an internally circulating fluidized bed with draught tube. But a little is different from J. Bi^[1].

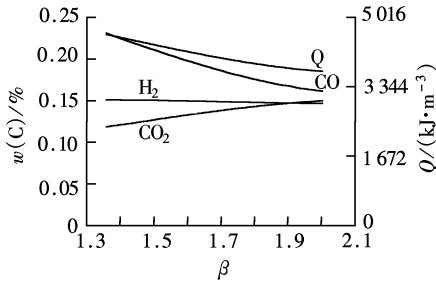


Fig.6 Effect of mass ratio of air to coal on CO,CO₂, H₂ and gas calorific capacity

Fig.7 is the effect of steam/coal mass ratio λ on compositions and gas calorific value. With the increase of the ratio, hydrogen and carbon dioxide increase and monoxide decreases. So steam-gas shift reaction plays an important role in compositions conversion. As to the hydrogen, its percentage changes little. With the increase of the steam flow, the temperature drops and gas calorific value decreases. According to the model, the most favorite steam/coal ratio is about 0.4 – 0.5. This is in good agreement with R. Govind^[4].

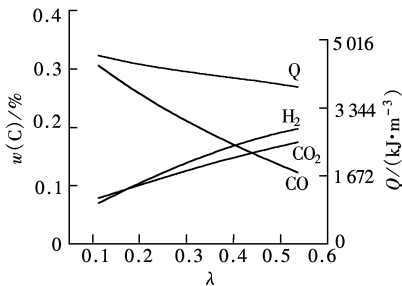


Fig.7 Effect of mass ratio of water to coal on CO,CO₂,H₂ and gas calorific

7 Conclusion

A model on a spouted-fluidized bed coal gasification is established and the numerical simulation is conducted. According to the result, gas composition in the spout zone changes drastically along the height. Gas exchanging between the spout and annulus has great impact on gasification. The composition in the freeboard keeps almost the same along height.

The pressure has great impact on coal conversion. High pressure is beneficial to the increase of gas calorific value. That is useful in carbonizer design. Increasing air and steam flow will decrease the gas calorific value.

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增压喷动流化床中煤半气化数值模拟

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摘 要 本文对增压喷动流化床中煤半气化进行了模拟,在模型中考虑了增压喷动流化床的物理特性、化学反应、能量平衡,对床压、床温、空煤比,汽煤比对生成煤气成分的影响进行了研究.计算结果表明增压喷动流化床中床压、床温对煤的半气化影响较强.

关键词 增压喷动流化床,煤气化,数值模拟

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