The Effects of Operational Parameters on the Transport Phenomena in COREX Melter–Gasifier

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Using a computational code developed for simulating the COREX melter–gasifier, the effects of operational parameters on the transport phenomena in the melter–gasifier were studied. The parameters studied were the bed height, C/O ratio, operating pressure and steam injection ratio. When the bed height was increased, the temperature near the combustion zone also increased due to there being sufficient heat exchange between the gas and solid phase. However, the freeboard zone temperature remained constant due to the increased residence time for heat exchange. Operational pressures affect the rate of tar in the coal. However, the extent of the change in the evolved tar as a function of pressure did not vary severely. The variation in the C/O ratio affected the heating rate of coal followed by a drastic change in the heat and mass transfer of solid and gas phases. The combustion zone and the freeboard zone temperature were changed largely by variations in the C/O ratio. The C/O ratio also changed the evolution rate of the coal by the changes in heating rate. From these considerations, the C/O ratio should be carefully controlled for the stable operation. The effects of steam injection into the melter–gasifier were also studied. Up to a steam injection rate of 30 %, the temperature of the combustion zone increased. Steam injection also affected the effluent composition of the gas phase. When the steam injection ratio was increased, the CO/CO₂ ratio was decreased while H₂/H₂O ratio was remained unchanged.

KEY WORDS: COREX melter–gasifier; computer simulation; operational conditions; bed height; C/O ratio; steam injection.

1. Introduction

The smelting reduction processes are known as an alternative to the blast furnace process. It has an advantage in flexibility of raw materials and operation restart etc. and a lower pollutant emission rate. Among them, the COREX process can be considered as the only commercial scale smelting reduction process. At the POSCO Pohang works, the COREX process has been successfully operated with 600 000 tons of pig iron production per year.

The COREX process is composed of two main reactors. One is a pre-reduction furnace that reduces iron ore by up to 90 %. Iron ore reduction is considered to occur mainly in this reactor. The other is melter–gasifier that finally reduces and smelts the iron ore and generates reducing gases by the combustion of coal for the pre-reduction furnace. Since the melter–gasifier gasifies coal and finally reduces and smelts iron ore, more complex chemical and mass transport phenomena, compared to the pre-reduction furnace, may occur in this reactor. The detailed description of the COREX process outlined in Ref. 1).

Generally, the COREX process uses raw ore and coal as a raw material and fuel, respectively. Therefore, mathematical modeling of coal pyrolysis behavior is essential for simulating the melter–gasifier.

To achieve stable operation and better performance, un-

derstanding of the transport behavior inside the reactor is essential. There are many approaches in understanding this behavior. Direct measurements of the reactor such as temperature, gas composition and pressure etc. are too difficult and expensive. Therefore a numerical study of the reactor based on the fundamental laws of physics and various conservation laws is considered as useful alternatives.

There is a paucity of publications relating to the COREX process. However, Shin *et al.*¹⁾ studied process modeling for the overall COREX process, which was mainly concentrated on process analysis. They did not include an analysis of the detailed transport phenomena. Lee *et al.*²⁾ developed a computational code for the COREX melter–gasifier. Using the developed code, they calculated the transport phenomena inside the reactor based on the mass and energy conservation laws and coal pyrolysis submodel. Their results had the advantage that they primarily studied the reactor using known physical laws. However, their study focused mainly on melter–gasifier transport phenomena at standard operating conditions that included coal pyrolysis behavior. The effects of operational parameters on the transport phenomena were not reported. This study has mainly concentrated on the effects of the operational parameters using the developed computational code for simulating the melter–gasifier.

The operational parameters considered in this study were the bed height, C/O ratio, operating pressure and steam in-

jection ratio.

2. Mathematical Modeling

The conceptual reaction zone of the COREX melter-gasifier is shown in Fig. 1. Coal particles over 8 mm fall from the top of the melter-gasifier and additionally, fine coal is injected from the dust burner. Pure oxygen is introduced from the tuyere and dust burner.

The governing equations and constitutive relations used in this study are listed in briefly in Table 1, which summarizes 192 ordinary differential equations used in this study. The equations presented are rather simple since they were formulated as balance equations. The complexity of these equations lay in the right hand side of the equations, which involve the heterogeneous char reaction as well as homogeneous reactions in the gas phase. Using these equations, the transport phenomena in the reactor were analyzed and the effects of each of the operational conditions were also studied.

As can be seen from the table, the transport properties of the coal, ore and flux mixture, and gas were calculated as separate phases. Firstly, coal is composed of volatile mate-

rials, moisture, ash and remaining char. For simulating the coal pyrolysis behavior, the FG-DVC (Functional Group-Depolymerization Vaporization and Crosslinking) submodel³⁾ was used. From the model, the mass of gas evolved and the elemental composition of the char remaining during coal pyrolysis was calculated.

The ore and flux mixture was assumed to be non-reactive with the coal and gaseous species. The ore and flux phase contributes only to the heat balance equations as chemically inert solid materials.

For the calculation of the gas phase continuity equations, five elemental continuity equations, which included C, H, O, N, S, and 22 species continuity equations were considered. The tarry substances, which are the by-products of the coal pyrolysis reaction, were treated as pseudo-gas species and were included in gas phase calculation.

The heats of reaction for the gasification and oxidation of the char were calculated by performing an energy balance around the particle-gas interface. The temperatures of the reactor product were assumed to have the same temperatures the char particles. As were the products of the heterogeneous reactions. The heats of reaction for the gasification reactions could be calculated in a similar manner.

The physical properties for calculating the conductivity, viscosity and diffusivity were quoted from Bird *et al.*⁴⁾ and Suuberg *et al.*⁵⁾ The full heat and mass transfer correlations are listed in the work reported by Lee *et al.*²⁾

Fig. 1. Schematic diagram of COREX melter-gasifier.

3. Numerical Integration and Assumptions

3.1. Numerical Integration

This system has the characteristics of a split boundary problem. This means the solid inlet value is known at the top of the furnace but information about the outlet value at the bottom of the furnace is lacking. On the other hand, gas inlet values at the bottom of the furnace are known. However, the outlet value of the gas phase at the top of the bed is not known. This problem may be overcome by separate calculations of the solid and gas phases until the convergence criterion is satisfied. In this study, the convergence criterion occurs when the temperature difference in the top of the bed between each iteration is less than 0.1 K. The

Table 1. Conservation equations for simulating the COREX melter-gasifier.

Solid Phase		Gas Phase	
$\frac{dW_{solid}}{dz} = -A \sum_{i=1}^6 r_i$	(i)	$\frac{dW_{gas}}{dz} = A \sum_{i=1}^6 r_i$	(ii)
$\frac{dh_{coal}W_{coal}}{dz} = A \left(-Q_{cg} - Q_{cw} - \sum_{i=1}^6 r_i H_{g,i} \right)$	(iii)	$\frac{dh_{gas}W_{gas}}{dz} = A \left(Q_{cg} + Q_{dg} - Q_{gw} + \sum_{i=1}^6 r_i H_{g,i} \right)$	(v)
$\frac{dh_{dri}W_{dri}}{dz} = A \left(-Q_{dg} - Q_{dw} - \sum_{i=1}^6 r_i H_{g,i} \right)$	(iv)	$\frac{dW_{g,l}}{dz} = A \sum_{i=1}^6 r_{i,l}^{gas}$	(vii-xxviii)
$\frac{dW_{moisture}}{dz} = -A r_{drying}$	(vi)	$\frac{dW_{g,j}}{dz} = A \sum_{i=1}^6 r_{i,j}^{gas}$	(xxix-xxxiii)
153 FG-DVC Model Equations		$\frac{dW_{tar}}{dz} = A \sum_{i=1}^6 r_d^{tar}$	(xxxiv)
		$\frac{dW_{tar,j}}{dz} = A \sum_{i=1}^6 r_{d,j}^{tar}$	(xxxv-xxxix)

$i = 1-6$ represents drying, devolatilization, CO₂, H₂, H₂O gasification and oxidation reactions respectively

$j = 1-5$ represents elements C, H, O, N, and S respectively

$l = 1-22$ represents 22 gaseous species considered in this code

Fig. 2. Calculation procedures for simulating the melter-gasifier.

freeboard zone and the combustion zone have no particulate phase. Their respective temperatures and compositions are calculated by the Gibbs free energy minimization method.⁶⁾

These calculation procedures are summarized in Fig. 2. The governing differential equations of the system using the one-dimensional assumption were integrated from the top to the bottom of the fixed bed together with a zero dimensional calculation of the freeboard and the combustion zone. In the initial calculation step, the gas temperature and mole fraction of the species presenting the gases were guessed on the top of the fixed bed. Using guessed gaseous properties, the solid phases were integrated and updated from the top to the bottom of the fixed bed using the LSODE (Lawrence Livermore Solver for Ordinary Differential Equations) package.⁷⁾ In the downward pass, the gas phase variables were held constant and the solid phase and solid-gas exchange quantities were calculated from the values predicted during the downward pass. When the integration reached the combustion zone, the solid phase temperatures and remained char compositions were used as input conditions for calculation of the combustion zone, which was calculated in advance by the zero dimensional assumption based on the balance equations. After completion of the combustion zone calculations, the gas phase temperature and gaseous species composition were used as the new initial input conditions for the calculation of the gaseous phase from the bottom to the top of the fixed bed. During upward integration, the gas phase properties and exchange quantities were updated and the solid phase properties held constant. When upward integration reached the top of the bed, the gas phase quantities at the top of the bed were then used as an initial guess for the next downward integration step. When the upward pass reached the top of the fixed bed, the freeboard zone calculation was initiated using the top gas temperature and composition and dust burner temperature and composition. These steps were carried iteratively until the convergence criterion was satisfied.

3.2. Assumptions

A steady 1-dimensional assumption was adopted for cal-

Table 2. The reference operating conditions.

Operating Condition	Value
Diameter of the melter-gasifier, m	7.3
Bed Height of the melter-gasifier, m	6.0
Operating Pressure, atm	3.0
C/O ratio, -	0.565
Temperature of Feed Coal, °C	750.0
Temperature of Feed Ore and Flux, °C	50.0
Temperature of Dust, °C	750.0
Temperature of Oxygen, °C	40.0
Temperature of Steam, °C	150.0
Coal 1 mass fraction	0.2
Coal 2 mass fraction	0.8
Flow rate of feed coal, kg/s	17.024
Flow rate of feed ore and flux, kg/s	27.133
Flow rate of Oxygen, kg/s	15.079
Steam injection rate, %	0.0
Particle diameter of coal, mm	12.0
Particle diameter of ore, mm	12.0
Heat Loss Rate, Watt	2.5085×10^7

culating the drying and devolatilization zone and the gasification zone. A steady zero-dimensional assumption was used for the freeboard zone and the combustion zone. The iron ore and fluxes were assumed to be chemically inert. Two types of coal were completely mixed in the melter-gasifier. The coal was burned to 100% at the combustion zone. Below the combustion zone, there was no char remaining. Finally the tar in the freeboard zone was fully decomposed into light gas species by the dust burner.

4. Results and Discussion

The results of the previous work,¹⁾ when comparing the calculated and experimental results, showed reasonably good agreement. However, their work mainly focused on the coal pyrolysis phenomena in the reactor at one operational condition. In this study, using the developed computer code for melter-gasifier, the effects of the operational parameters on the transport phenomena in the reactor were analyzed.

Table 2 summarizes the reference conditions for used in these calculations. In the table, the bed height, operating pressure, C/O ratio and steam injection ratio was treated as manageable operating parameters. Heat loss rate is maintained constant for comparing other results to reference conditions.

4.1. Bed Height

In the real operation, the bed height was regarded as the most important operational parameter that operation engineers can manage. If the temperature of the pig iron decreases, it can be increased by setting the bed height higher and *vice-versa*. Therefore, the pig iron temperature can be controlled by changing the bed height. However, this operational control was not based on any understanding of the transport phenomena. A detailed mechanism of the transport phenomena of the reactor is essential in understanding the behavior of the reactor and improving performance.

The temperature variations of the ore and flux mixture with various bed heights are shown in Fig. 3. As the height

Fig. 3. Ore and flux temperature variation in the bed with bed height.

Fig. 4. Gas phase temperature profiles with bed height in the bed.

of the bed increases, the temperature of ore and flux shows larger differences near the combustion zone than in the upper zone of the bed. In the case of a 5.5 m bed height, the ore and flux mixture is not melted completely near the combustion zone. As a result, the temperature of the pig iron from the hearth is predicted to show a lower temperature due to incomplete melting of the iron ore. This might cause instability in the process. On the other hand at a bed height of 6.5 m, the ore and flux mixture temperature showed higher temperature profiles than the lower bed. However, the temperature of the melter-gasifier should be maintained for stable operation. This could result in the need for additional cooling agents and increased production cost. However, in both cases the temperature profiles show almost the same gradient. From these considerations, the differences in bed height are affected mainly by the level of heat exchange between gases and solid phases and rarely have an effect on the heating rate of the solid phase.

Figure 4 shows the temperature variations of the gas phase as a function of the bed height. Here it can be seen that the higher the bed, the higher the temperature of the gas phase. This may be explained as follows: The level of heat exchange between the gas and solid phase are larger in the higher bed due to the longer residence time of the solid and gas phase. The solid phase receives more heat from the gas phase. This causes an increase in solid phase tempera-

Fig. 5. Combustion zone and freeboard zone temperature variation with bed height.

ture. The increased solid temperature raises the temperature of the combustion zone. In turn, the increase in the combustion zone temperature also raises the gas phase temperature of the bed. As a result of the successive heating processes, the overall temperature of the reactor is increased.

Figure 5 compares the temperature of the combustion zone and the freeboard zone as a function of bed height. The combustion zone temperature is raised as the bed height increases. As the bed height increases, the temperature of the solid phase entering the combustion zone is also increased, which is the reason why the combustion zone temperature increases. However, the temperature of the freeboard zone remains constant. The factors that determine the temperature of the freeboard zone are temperature and composition of the gas phase from the bed top, coal fine particles and oxidizer injected from the dust burner and the level of tar entering the freeboard zone. Though the overall temperature of the bed was raised, the gas phase sufficiently transferred its enthalpy to the solid phase. As a result, the gas temperature at the top of the bed shows large variations. In addition, the temperature of the gas phase entering the freeboard zone remained almost constant, thus the temperature of the freeboard zone is unchanged.

4.2. Operating Pressure

For stable operation, the evolved tar should be completely decomposed to light gas in the freeboard zone. The amount of tar that evolves during the coal pyrolysis process can be affected by the operating pressure. Figure 6 shows the amount of evolved tar as a function of operating pressure. As can be seen, the level of tar decreases with increasing operating pressure. The tar evolved from the coal to the gas phase undergoes diffusion and convection in and around the coal particle. The operation pressure can be thought of as a suppressor of the diffusion and convective transfer of the tarry substances in and around the coal particle. Under the same operating conditions, by increasing the operational pressure, the tar evolution rate might be controlled.

4.3. C/O Ratio

Generally, the reactor operation is primarily determined from the mass balance of carbon and oxygen. Carbon

Fig. 6. Tar flow rate variation with operating pressure.

Fig. 8. Ore and flux temperature profiles with C/O ratio.

Fig. 7. CO mole percent variation with C/O ratio in the bed.

sources in the melter-gasifier are composed of two parts. One is from the top of the melter-gasifier by gravitational force as a lump. The other is from the dust burner in the form of fine particle together with oxidizer gas. A minor source of carbon is carbon deposited on the reduced iron. In this study, the mass of deposited carbon was considered to be negligible compared to carbon from the lump and fine coal. Oxygen in the reactor was mainly originated from the tuyere. Another source of oxygen is the dust burner. The ratio of carbon to oxygen heavily affects the overall temperature and composition of the gas and solid phase in the reactor. In the following, the effects of the C/O ratio will be discussed.

At the reference condition, the C/O ratio is set to 0.565. If only C and O exist in the reactor, the composition of the effluent gas is mainly CO_2 with a small amount of CO. However, due to hydrogen, which combines with carbon to form hydrocarbons, the reactor effluent gas composition shows larger concentrations of CO.

If C/O ratio increases, which can be changed by coke bed height or oxygen injection rate, the CO concentration increases due to the thermodynamic considerations. This means that larger amounts of reducing gas are generated and the effluent has a larger reducing potential. Therefore, larger amounts of CO generation are preferred in view of reduction capacity. Figure 7 shows the CO gas mole fraction variation with various C/O ratios. CO becomes the dominant chemical species with increasing C/O ratio near

the combustion zone. This means that the carbon fraction at the combustion zone is increased. As the gas phase ascends from the bottom to the top of the bed, the mole fraction of CO in the gas phase reduces due to coal pyrolysis, which evolves large amounts of light gas, especially H_2 . However, the tendency for a high C/O ratio to have a high CO mole fraction was maintained. In the viewpoint of generation of reducing gases, a higher C/O ratio is favorable.

Figure 8 shows ore and flux temperature variations with various C/O ratios. From the figure, the solid phase temperature is over 2500°C . This is caused by the following reasons. For analyzing the effects of specific operational condition, other parameters that might be lower the solid temperature should maintain constant in the simulation. This caused a high temperature of solid phase. A higher C/O ratio shows a low ore and flux temperature, which is due to the following reasons: The low C/O ratio means that smaller amounts of carbon fall into the combustion zone. The carbon reacts with relatively large amounts of oxygen. Because the CO_2 forming reaction emits more enthalpy than the CO forming reaction, the temperature of the combustion zone is increased. This results in an overall increase in the gas and solid phase temperature in the reactor. This should not be preferred in terms of production cost. On the other hand, a higher C/O ratio shows relatively low ore and flux temperature profiles. Below a C/O ratio of 0.575, iron and ore flux do not completely melt in the bed and fall into the combustion zone, which may make the process unstable. Thus, an optimum C/O ratio should be carefully chosen and should be maintained at a constant in the reactor to enable stable operation.

The mass loss rate of coal with various C/O ratios is shown in Fig. 9. The coal mass loss rate shows different profiles compared with bed height variations. The coal mass loss rate profiles as a function of the bed height are not presented here. This is because it only shows a shift in the profiles as the bed height increased. As the ratio decreases, the peak point of mass loss rate moves toward the top of the bed and the absolute rate is increased. Unlike the bed height variation, this is thought of as a change in the heating rate of the coal in the reactor. The peak point shift might be thought as the result of a change in heating rate. Coal with a higher heating rate evolves larger amounts of light gas and tarry substances. As a result, the amount of

Fig. 9. Coal mass loss rate variation with C/O ratio in the bed.

char remaining decreases and the amount of carbon falling into the combustion zone also decreases. This significantly changes the reaction condition in the combustion zone.

The C/O ratio variation also affects the temperature of the freeboard zone. The temperature of the freeboard zone with increasing C/O ratio decreases although there is a less evident effect when compared to the combustion zone. When the C/O ratio is greater than 0.575, the temperature of the freeboard zone falls below under 1000°C which is thought of as the lower limit of the tar decomposition reaction. Below this temperature, tar does not completely decompose. Remaining tar condenses on the reactor wall when the gas cools to a specified temperature. In online operations, the exact control of the C/O ratio is crucial for the stable operation.

4.4. Steam Injection

Since the COREX process has been operating at the POSCO Pohang works, which has a well-known integrated mill, there are always excessive amounts of steam. If steam is injected into the melter-gasifier, the larger amount of reducing gas which contains more hydrogen gas may be generated. Since, hydrogen gas is environmentally friendly, its usage may increase.

As injected steam has a higher heat capacity and lower temperature than the combustion zone, the transport phenomena in the melter-gasifier may be disturbed by the steam injection.

Figure 10 shows ore and flux temperature variations with various steam injection rates. The steam injection ratio was calculated from the relative molar concentration of hydrogen to the total carbon in the melter-gasifier. Furthermore, the temperature of the steam injected from the tuyere was maintained at 150°C which is higher than the injected oxygen. At steam injection rate of 30% or below, as the amount of steam increases, the ore and flux temperature increase. This was thought to be the result of the following: Steam injection had two opposing effects on the heat and mass balance of the combustion zone. Since relatively low temperature gas is injected into the combustion zone, it has a tendency to lower the temperature of the zone. However, in the viewpoint of mass balance, injected steam causes a

Fig. 10. Ore and flux temperature profiles with various steam injection rate.

Fig. 11. Gas compositions of the freeboard zone with various steam injection rate.

decrease in the C/O ratio. This causes the temperature of the zone to increase. As can be seen from the figure, up to 30% of the steam injection rate, the temperature of the zone has a tendency to increase due to the dominated the decrease C/O ratio. However, at an injection rate over 30%, the decreasing tendency dominates.

Since one role of the melter-gasifier is to generate the reducing gas for the pre-reduction furnace, the effect of the effluent gas composition with the steam injection rate should be considered. The gas composition of the freeboard zone with the various steam injection rates is showed in Fig. 11. As the steam injection rate is increased, the CO mole fraction is decreases linearly with the other species increasing linearly. This can be predicted from the C/H/O ratio of the reactor since the reduction rate of iron ore is generally governed by the difference between reactant and product gas mole fraction, *i.e.* ($C_{\text{reactant}} - C_{\text{product}}$), where C represents molar concentration (mol/m^3) of the gas phase. The difference between CO and CO_2 decreases and H_2 and H_2O is maintained at a constant. Since iron ore reduction by CO and H_2 was an equilibrium reaction, the change in the ratio of reactants to products might severely affected the overall reduction process. If the ratio is decreased, the iron ore reduction rate might also be slowed even though the absolute amount of injected gas is increased. When steam is

injected into the melter–gasifier, although its increased usage has an advantage in lower pollutant emission, the rate should be carefully chosen when considering the decrease in gas phase reduction potential.

5. Concluding Remarks

Using the developed computer code for simulating the melter–gasifier, the effects of the various operational conditions on the transport phenomena of the reactor were studied.

In this study, the bed height, operational pressure, C/O ratio and steam injection rate were considered as operational parameters.

Bed height variations may influence the combustion zone temperature. As a result of sufficient heat exchange between gas and solid phase, the freeboard temperature remains constant. However, the overall temperature profile of the reactor moves upward due to an increase in combustion zone temperature.

The operating pressure can affect the tar evolution rate in the coal. However, in this simulation, the change in the evolution rate did not vary much.

The reactor C/O ratio has been considered as one of the more important operational parameters. A C/O ratio variation can affect the overall heat and mass transport phenomena. The temperature of the combustion zone and the freeboard zone were changed largely by variations in the C/O ratio. C/O ratio variation also changed the tar evolution rate, coal heating rate, overall reactor temperature and the gas phase composition. For stable operation, the C/O ratio should be carefully controlled.

Steam was used for generating additional reducing po-

tential. Steam affected the transport phenomena of the combustion zone in two ways. One is the heat balance of the zone due to the temperature difference of the steam and the zone. The other is the mass balance of the zone. As a result of the two competing effects, the combustion zone temperature was determined. At steam injection rates below 30%, the temperature of the combustion zone increases. The composition of the freeboard zone is also changed. The amounts of CO decreased linearly and the other species increased linearly with the increase of the steam injection rate. The change in the ratio of the reactant to product was predicted to severely affect the kinetics of the iron ore reduction process. Therefore, the steam injection rate should also be carefully chosen for the stable operation.

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