THERMODYNAMIC MODELLING OF COREX MELTER GASIFIER USING FactSage™

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Abstract: Coke is the fuel used for iron making in conventional process routes like blast furnace. COREX is one of commercially proven alternative iron making routes developed by researchers to produce hot metal from iron ore directly using coal, in cost effective and environmental friendly manner. COREX is two stage smelting reduction process, which consists of reduction shaft placed above the melter gasifier. Melter gasifier completes the reduction and smelting of pre reduced ores from reduction shaft, along with coal gasification. Although 100% replacement of fuel requirement by coal is not possible and some amount of coke is also charged in Corex process depending upon the quality of coal affordable by industries. Present work investigates such possibilities with the help of a thermodynamic model of Corex melter gasifier using FactSage macro-programming approach. The resulting mathematical model not only predicts the weights and compositions of hot metal, slag and top gas but also studies the effect of degree of metallization on coal/coke consumption.

Keywords: Smelter gasifier, FactSage™, metallization, fuel utilization

1. Introduction

COREX is one of the commercially established smelting reduction processes to produce molten iron of the blast furnace grade from the iron ores. It (formerly known as KR method) was initially developed by German Korf Company and VAI in late 1970s[1]. The process consists of two reactors namely reduction shaft and melter gasifier as shown in Figure 1. The iron ore gets pre-reduced to wustite in reduction shaft and transported to melter gasifier where final reduction of wustite takes place and molten metal is tapped. The reduction gas being generated in the melter gasifier is recycled through the cyclone to the reduction shaft for pre-reduction. The percentage of the reduction gas being recycled, based upon the CO/CO_2 ratio of the gas, decides the efficiency of the process.

The comprehensive model of the process, which can predict the input parameters based on the raw material quality, was a challenge to the researchers. Koria et al.[2,3] has studied the influence of post combustion ratio and degree of metallization through a static thermochemical model. Qu et al.[4] has developed a comprehensive static model of COREX, which was restricted to species balance of Fe, slag, MgO, and Al2O3. The coal and coke fed to the process is known to be used for reduction and smelting. The fractions of coal and coke utilized for reduction and smelting will help to understand the process in depth. A thermodynamic model for the COREX melter gasifier was developed by Srivastava et al.[5]. This model tries to predict the hot metal and slag composition for different degrees of metallization, with raw material quality as inputs. This model also contains a simplified coal pyrolysis module for smelter gasifier.
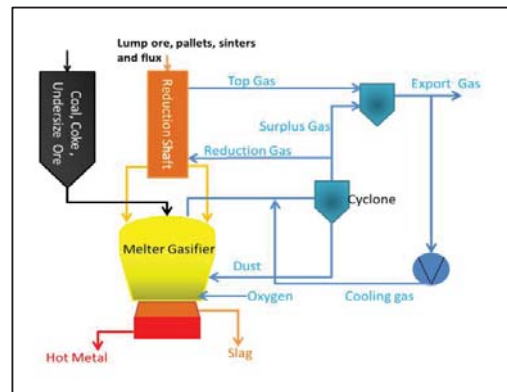

Figure 1 COREX Process

The present work is a study on the effect of fractions of coal and coke utilized for reduction and smelting respectively. The present thermodynamic model has been developed using FactSage macro program. The model divides the melter gasifier into different equilibrium zones and tries to perform material balance in each zone and overall heat balance. The model predicts the output quantity and composition of hot metal, slag and exit gas for given set of operating conditions and raw material quality.

2. Thermodynamic model

The smelter gasifier of the Corex process was modeled thermodynamically. The melter gasifier of COREX was divided into six equilibrium /

stoichiometric reactors, namely A, B, C, D, E, and F, have been considered in the model described in flow chart shown in Fig. 2. The free energy minimization principle with the help of FactSage 6.4 software (CRCT, Montreal, Quebec, Canada)[6] was used for all computations in the various reactors involving their inputs. The overall heat balance was performed at the end of calculation. FToxid, FTmisc, and FactPS databases were selected for the calculation. FToxid, FTmisc, and FactPS solution and compound databases contains the data for oxide solutions, dilute liquid alloys and pure substance and all stoichiometric solid and liquid oxide, dilute liquid alloy compounds evaluated/optimized by the FACT group[7].
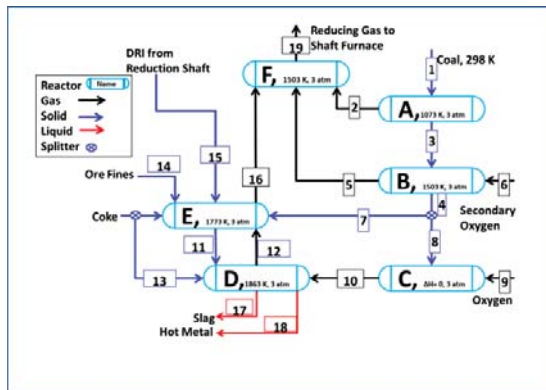

Figure 2 Flow Sheet of the Macro Program

Coal pyrolysis and gasification phenomena, has been dealt by three reactors (reactor A, B, and C) whereas the other two reactors (reactor D and E) deals with the reduction and smelting of directly reduced iron (DRI). Reactor F has been considered for the equilibration of gas streams of reactors A, B and E. The inputs to the model as obtained from plant data of JSW steel's COREX plant:

(i) Ore Composition (in %): Fe_2O_3: 90.36%, Mn: 1.07%, P_2O_5: 1.60, FeS: 0.01%, SiO_2: 4.42%, Al_2O_3: 2.56%

(ii) Raw Materials (kg/THM): Ore Pellets: 1340, Ore fines: 141, Flux: 330, Coal: 900, Coke: 222

(iii) Temperature: Coal: 298 K, Coke: 298 K, Oxygen: 298 K, DRI: 1503K

The temperature and pressure of these reactors obtained from work of Srivastava et al.[5].

(iv)Reactor Temperature: A: 1073 K, B: 1503 K, C: Adiabatic Calculation, D: 1863 K, E: 1773 K, F: 1503 K.

Reactors A, B, and F represents the free board zone, where devolatilization of coal, decomposition of volatile matter, dust burning, and partial gasification the char occurs. Reactor A performs drying and primary pyrolysis reactions. Reactor B deals with the burning of carbon with oxygen to form a dust burner. The reacted char obtained from reactor B undergoes adiabatic combustion in the reactor C (adiabatic reactor). The temperature of this reactor is computed from the adiabatic conditions requirement. Reactor E receives metallized DRI from reduction shaft, which is reduced by coke fed into this reactor (E). The reduced charge obtained from the reactor E is smelted in the reactor D along with coke to produce the hot metal and slag. Reactors E and D are arranged sequentially to simulate the counter current flow between solids and gases. One more reactor, reactor F, has been considered which equilibrates the gas output streams of reactor A, B, and E.

3. Simulation

The model algorithm considers two splitters, namely for coke and coal, as shown in Fig. 2. The coal char stream 4 from Reactor B splits for direct reduction (E) and combustion (C) as stream 7 and 8, respectively. The coke charged in melter gasifier is also splitted into stream 13a and 13b, for direct reduction (E) and smelting (D) of ore. The splitter for coke and coal were varied individually to study the effect of the fraction of utilization of coal and coke for reduction and smelting. The term "coal ratio" is defined as the fraction of dry devolatized coal utilized for combustion and "coke ratio" is defined as the fraction of coke consumed for smelting.

4. Results and Discussions

4.1 Influence of degree of metallization:

The influence of varying degree of metallization from 10% to 99 % on slag, utilized gas after direct reduction, solid after direct reduction, and reducing gas are plotted in Figure 3. Other process parameters were kept constant as obtained from the JSW COREX plant. The ratio of coke for smelting was taken as 0.5, and ratio of coal char for combustion was taken as 0.9.

The slag generated decreases gradually from 455 to 418 kg with the increase in degree of metallization from 10% to 80% as shown in Fig. 3(a). On further increase in degree of metallization the amount of slag produced remains constant. Opposite trend is observed for the direct reduced ore coming from Reactor E as shown in Fig. 3(c), which remains zero up to 80% degree of metallization, starts increasing and reaches 200kg on further increase. The gas from direct reduction decreases with increases in degree of metallization from 1000 to

750 kg, as shown in Fig. 3(b), which can be attributed to low amount of iron oxide in highly metallized output of reduction shaft.
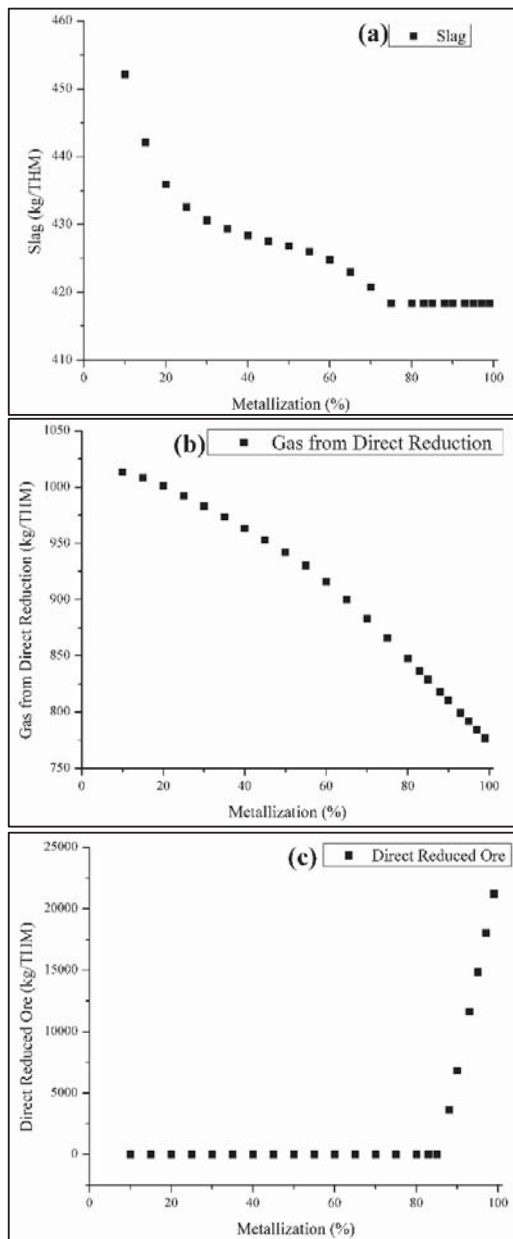

Figure 3: Influence of degree of metallization on amount of (a) Slag, (b) Gas from direct reduction, and (c) Direct reduced Ore

4.2 Influence of coal ratio

Similar study was performed for coal ratio, the degree of metallization was kept constant at 90% and coke ratio was held at 0.5, thus providing equal coke for direct reduction and smelting. The coal ratio was varied from 0.01 to 0.99. The influence of this variation was studied on total reduced ore

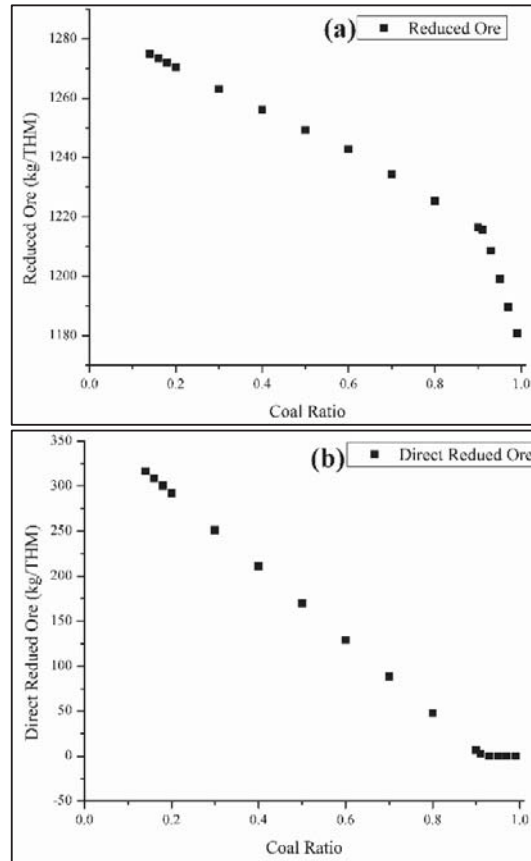mass, combustion gas, combustion char, and direct reduced ore.

Figure 4: Influence of coal ratio on (a) total reduced ore and; (b) direct reduced ore quantity

Total mass of reduced ore decreases gradually from 1280 kg to 1180 kg for increase in ratio of coal for combustion from 0.14 to 0.99, as shown in Figure 4(a). It is noticed from Figure 4(d), the amount of reduced solids by direct reduction decreases with higher ratio of coal diverted for coal combustion. At higher ratios of 90% of coal being available for combustion no direct reduction is feasible. This reason cause to steep change in amount of total reduced ore for less than 10% of coal is made available for direct reduction.

Gas evolved during combustion increases from 600 to 1100 kg as the higher ratio of coal is combusted as shown in Figure 5(a), which leads to higher amount of combustion products from 100 kg to 220 kg, as observed from Figure 5(b).

4.3 Influence of coke ratio

The degree of metallization was kept constant at 90% and coal ratio was kept constant at 0.9. The coke ratio was varied from 0.01 to 0.99. The

response of this variation was recorded for amount of direct reduced solid, as shown in Fig. 6.
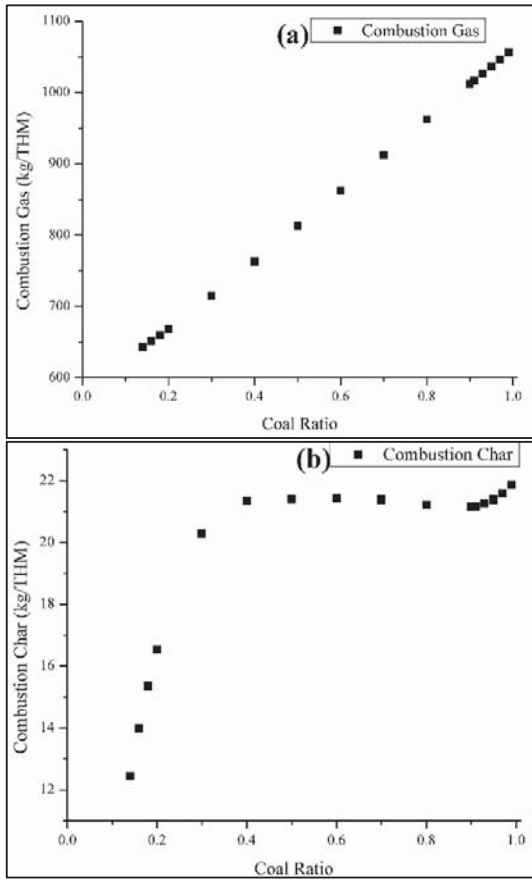

Figure 5: Influence of coal ratio on (a) Combustion gas and; (b) Combustion char quantity

Figure 6 shows that the amount of direct reduced solid decreases with increase in ratio of coke supplied for smelting. This behavior is due to unavailability of carbon for direct reduction. If more than 60% of the total coke is used for smelting, then the no direct reduction of ore takes place, as entire solid will be reduced in the previous stages, using the gas generated from combustion of coal.

5. Conclusions

The thermodynamic model of Corex melter gasifier has been developed using FactSage™. The fraction of coke divided between direct reduction and smelting was varied and its influence on output

parameters were studied. The degree of metallization should be more than 80% for direct reduction, which utilizes the gas effectively, increase direct reduced ore from 0 to 21300 kg/THM. As the amount of coke charged in the process is 20% of total fuel charged, its effect was negligible on other output parameters except on the mass of direct reduced ore. This indicates the complete reduction by gases in previous stages, for more than 60% coke used for smelting. The fraction of coal made available for combustion was varied and its effect on the other output parameters were studied. As the coal available for combustion increases the combustion products also increases twice (12 to 24 kg/THM of char) which later help in reduction of ore by gas and decreasing the amount of direct reduced ore to 325 to 0 kg/THM.
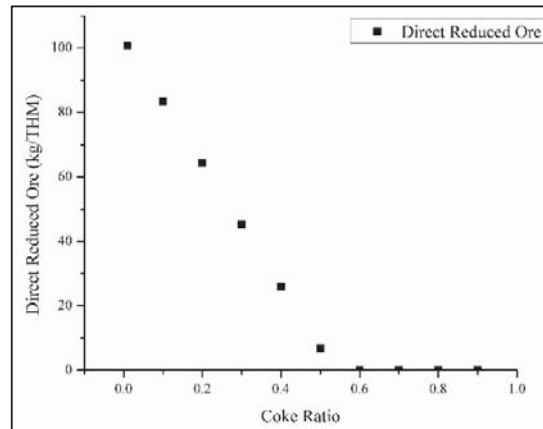

Figure 6: Influence of coke ratio on amount of direct reduced solid

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