

Simulation of the Iron Smelting-Reduction Process

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ABSTRACT

A computer program is developed to simulate a two-step smelting-reduction process. Laws of thermodynamics, kinetics, iron-oxide reduction, energy balance, materials balance and transfer of heat and mass between metal, slag and gas are taken into account for development of the model. Local equilibria between metal and slag according to the quadratic formalism of the regular solution model is considered. Dissolution of iron and its oxides in the molten slag and heat transfer from post combustion gases to the molten bath are numerically analyzed. The model is able to evaluate the effect of all important variables on productivity and effectiveness of the process. Special attention is paid to the operational conditions of the reduction furnace while working with the gases coming from a smelter with a high post-combustion ratio and a high reducing-power produced through reforming of the off-gases of the smelter with a natural gas stream in order to minimize the total energy consumption and to maximize the productivity. The application of the model to optimize the behavior of a two stage smelting-reduction system is investigated.

1. INTRODUCTION

Designing a continuous reactor for production of liquid metals has several advantages of (1) increasing production rate to size ratio, (2) reduction of capital costs, (3) increasing feasibility of construction of small scale melting units, (4) drastic reduction of the costs of transportation, handling and storage of both semi-finished and finished materials, and (5) possibility of direct utilization of original raw materials¹.

The process has, however, certain difficulties concerning (1) low-speed kinetic processes, (2)

low-grade refractory materials, (3) unefficient heating facilities and (4) problems associated with dynamic process system design and control^{2,3}.

A multi stage semi continuous system can, however, be considered as an intermediate solution with lower number of difficulties. Direct smelting of iron is a good example comprising of two consecutive units for pre-reduction and heating and melting processes. Considerable attention have been paid during past 15 years to this method^{4,5}. There are, however, a number of shortcomings that must be resolved through further research.

Operational efficiency of the system is influenced by such variables as shape and geometry of the vessels, method of charging, rate of feeding, analysis of materials, size of particles, use of alternative fuels and their feeding rate, flow rate of gases blown into the vessel and quantities of impurities that come with charge materials into the bath. Effects of these parameters can be determined through evaluation of mass and heat balances, thermodynamics and kinetics of homogeneous and heterogeneous reactions and flow of fluids within and inbetween the phases.

Investigation of these effects is both difficult and expensive if it is aimed to be performed under real practical conditions. Bench scale experimental work is also usually not feasible. Many investigators have therefore simulated the process through application of the physico-mathematical models that may be capable to predict the influence of the important variables⁶⁻⁸.

There are drastic shortcomings, however, that may inflict these models due to the complexities and lack of thermo-chemical data. Ideal solution behavior is, for example, a common assumption made by almost all previous investigators. Practical constraints due to the limited reaction kinetics is generally ignored and constant values are pre-assigned to the influential variables such as HTC (Heat Transfer Efficiency), PRD (Pre-Reduction Degree) and PCR (Post Combustion Ratio). These are not, however, independent of the rates of consumption of coal, transfer of heat and kinetic processes that occur in the direct smelting reactors.

Regardless of the complexities raised due to the interrelation of the changes and effects, use of computer simulation can facilitate a precise quantitative treatment of the subject. A regular solution model with quadratic formalism can be employed to evaluate balances of materials and energy together with the thermodynamics and kinetics of the reactions⁹. Efficiency of transfer of heat and mass can be evaluated from reaction kinetics and heat balance calculations^{10,11}.

In this study, a combined double-vessel process is considered with special attention being paid to

geometric design, productivity, effectiveness, energy optimization and economics of the process. Optimum conditions for acquiring the maximum efficiency in heating, reduction, melting and purification of the metal until achieving the desired chemical content can be predicted by application of the model to the special circumstances of interest.

Effective transfer of heat from post combustion reactions, possibility of utilization of both scrap and pre-reduced ore, addition of alternative fuels, estimation of height of foamy slag, continuous desulfurization and decarburization reactions, evaluation of chemical analyses of the products, presumption of variable geometry and design for pre-reduction reactor and calculation of productivity of the process all are considered in the model.

2. MODELING

Schematic illustration of the double vessel

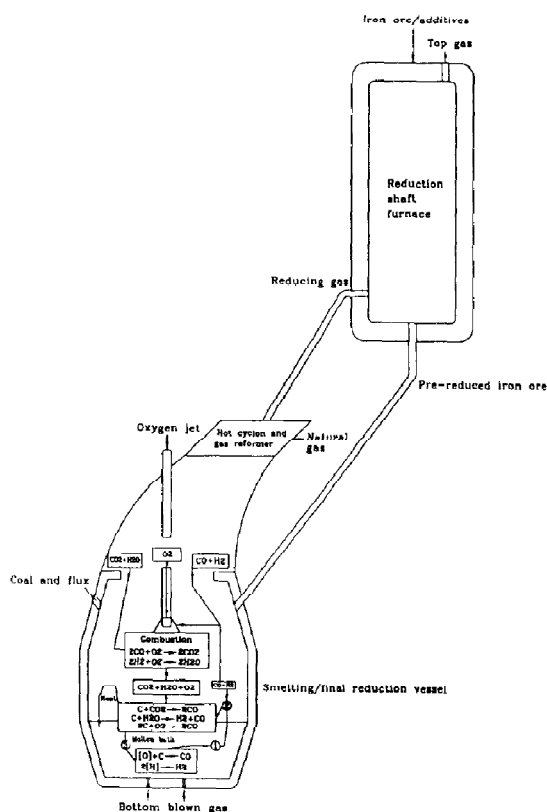


Figure 1. Schematic illustration of double-vessel system used in this research.

pre-reduction/smelting system used in this investigation is shown in Figure 1. The heat that is required for the smelting process is principally provided from oxidation of the coal particles charged into the furnace. The combustion process is performed at the upper part of the smelter. Released enthalpies of the reactions are principally transferred into the molten bath. Reforming of the off-gas can be achieved with employment of a hot cyclon and reformer box that can be installed between the smelter and the pre-reduction vessel. The pre-reduction vessel is employed to provide the pre-reduced materials required to be fed into the smelter.

A stream of natural gas may be injected into the reformer box. Reforming reactions can end-up with an enriched out-flow. Utilization of the out-flow in lower section of the pre-reduction vessel results in formation of a highly metallized burden. Geometry and design of the pre-reduction vessel can be changed as a function of the reduction potential and rate of the reformer out-flow.

The first approximation for evaluation of the rates of consumption of materials and energy can be practiced through presumption of unknown system variables such as PRD, HTC, gas temperature (T_g) and coal weight. Partial pressure of the gases are determined from PCR and the equilibrium constant of the reactions occurring in the gaseous phase:

$$PCR = 100 \left(\frac{P_{CO_2} + P_{H_2O}}{P_{CO_2} + P_{H_2O} + P_{CO} + P_{H_2}} \right) \quad (1)$$



The activities of the components of the slag are determined from quadratic formalism of the regular solution model modified by a "conversion free energy" term ΔG^o :

$$RT \ln \gamma_i = \sum_j \alpha_{ij} X_j^2 + \sum_j \sum_k (\alpha_{ij} + \alpha_{ik} - \alpha_{jk}) X_j X_k \quad (3)$$

γ_i : Activity Coefficient of component i of slag

α_{ij} : Interaction Energy of Cations

X_j : mole fraction of component j of slag

$$RT \ln a_i = RT \ln a_i(R.S.) + \Delta G^o \quad (4)$$

a_i : Activity of component i of slag

$a_i(R.S.)$: Activity of i based on regular solution model

The activities of the components of the metallic phase are determined from first and second interaction parameters¹³. Assuming equilibrium between liquid iron and FeO of the slag, the oxygen content of the molten metal is determined from¹⁴:

$$\%O = 0.6867 \Lambda + 0.00296 \%FeO + 0.5106 \quad (5)$$

$\%O$: oxygen content of molten metal

Λ : optical basicity of slag

The quantities of the conversion free energy, the free energies associated with the interaction between the cations present in the slag, the optical basicity of the pure oxides and the first and the second order interaction parameters are listed in Reference 15.

The sulfur content of the slag, (%S), is determined based on optical basicity equations¹²:

$$\log (\%S) = 0.5 \log \left(\frac{P_{S_2}}{P_{O_2}} \right) - 13.913 + 42.84\Lambda - 23.82 \Lambda^2 - \frac{11710}{T} - 0.0222 (\%SiO_2) - 0.02275 (\%Al_2O_3) \quad (6)$$

$$\Lambda = \sum N_i \Lambda_i \quad (7)$$

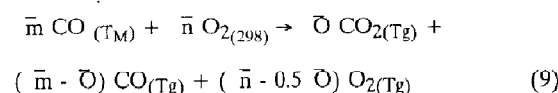
N_i : Equivalent Fraction of Cation i in slag

Λ_i : Optical Basicity of Pure Oxide of Cation i

$$N_i = \frac{n_i x_i}{\sum n_i x_i} \quad (8)$$

n_i : Number of Moles of i in Compound

For modeling of the post-combustion process, oxidation of CO is considered according to:



in which \bar{m} is the flow rate of CO produced at T_M in the reactor and \bar{n} is the rate of blowing of oxygen into the reactor at 298°K, etc. These rates are determined from mass and heat balances in the reactor.

Particle distribution in the gas phase is evaluated from⁷:

$$R_v = 100 \exp \left[-\left(\frac{d}{d'} \right)^a \right] \quad (10)$$

In which R_v is mass percentage of droplets with diameters larger than d , and d' is the minimum diameter of the suspended drops. The heat transferred from the gas into the descending droplets can be evaluated from the dynamic behavior of the system. The suspension time of the droplets ($2t_f$) and their descending speed (u) are determined from numerical solution of the following equations:

$$-\frac{1}{6} \pi d_D^3 \rho_D \frac{du}{dt} = 3 \pi d_D \mu_G (u_G - u) + g \rho_D \frac{1}{6} \pi d_D^3 \quad Re \leq 1 \quad (11)$$

$$-\frac{1}{6} \pi d_D^3 \rho_D \frac{du}{dt} = -\frac{3}{2} \pi \mu_G^{1/2} \rho_G^{1/2} d_D^{3/2} (u_G - u)^{3/2} + g \rho_D \frac{1}{6} \pi d_D^3 \quad Re > 1 \quad (12)$$

The coefficient of transfer of heat is determined from the correlations between the dimension-less quantities Nu, Pr and Re. The total quantity of heat

that transfers into the drops (\bar{Q}_t) is evaluated from micro-kinetics of the heating process:

$$\bar{Q}_t = \sum_i \frac{6 \bar{M}_D v_i}{\rho_D d_{D,i}} \int_0^{t_{r,i}} (h_{r,i} - h_{c,i})(T_G - T_{D,i}) dt \quad (13)$$

This heat comes from combustion of the gases (Reaction Number 9) and is dependent upon macro-kinetics and thermodynamics of the reactions occurring between solid, liquid and the gas phase. Efficiency of transfer of heat from gas into the molten bath is evaluated from:

$$HTC = \frac{\bar{Q}_t}{\bar{Q}_{t,l}} \quad (14)$$

in which $\bar{Q}_{t,l}$ is the total heat that is generated by the combustion reaction.

The degree of pre-reduction of the burden can be evaluated from the thermo-chemistry of the gas-solid reactions. Differential equations describing multi-stage counter-current plug-flow inside the pre-reduction vessel are numerically solved to evaluate temperature and the composition of gas and solid materials both locally and globally.

Evolution of the gases emanating from the liquid phase results in production of a foamy slag. The height of the slag is related to both the physical properties of the slag and velocity of the gas^{16,17}:

$$H \propto \frac{\mu_s}{(\rho\sigma)^{1/2}} \cdot \frac{Q}{A} \quad (15)$$

H: Height of Foamy Slag

μ_s : Viscosity of Slag

ρ : Density of Slag

σ : Surface Tension of Slag

Q: Flow Rate of Slag

A: Surface Area of Molten Metal pool

Detailed descriptions of the properties and their evaluation methods are given in References 18, 19 and 20.

The overall process undergoes a number of constraints. Large volumes of gas, for example, cause the formation of an extra ordinary foamy slag that can raise the height of the bath and cause a lowering in the smelter's productivity. Excessively high degrees of metallization, on the other hand, causes lowering of the height of the bath and decreasing the energy efficiency of the system.

The productivity can also be influenced by extent and mechanisms of the reduction reactions, transport of mass and momentum within and inbetween the phases, dissolution and final reduction of the oxides and removal of the impurity elements from the metallic phase²¹. An example is the rate of reduction of liquid FeO which depends on the iron content of the slag phase²²:

$$\bar{R} = k \cdot \%Fe \quad (16)$$

\bar{R} : Semi-steel Production Rate

The rate constant k depends on the amount of agitation in the bath, temperature and volume of the slag and weight of carbon particles suspended in the liquid phase²³:

$$k = k_1 + \left(\frac{W_s}{A}\right) \cdot \left(k_2 + \frac{W_c}{W_s} k_3\right) / 1000 \quad (17)$$

k_1 , k_2 and k_3 are empirical quantities measured by previous investigators²³.

The thermodynamic data required for calculations are obtained from References 24, 25 and 26. The transport properties are given in References 7, 15 and 27. The flow chart of the simulation model produced in this research is illustrated in Figure 2.

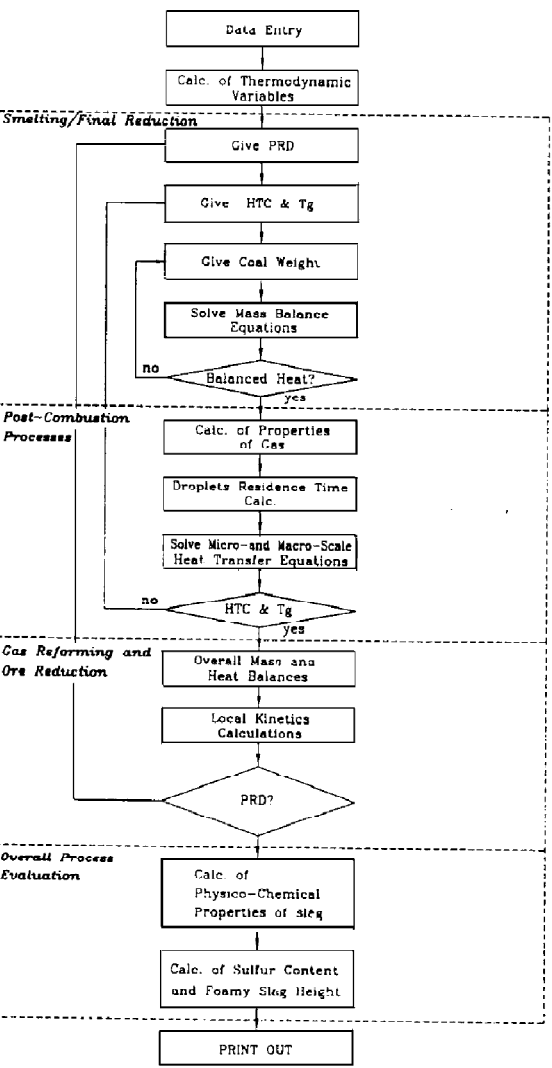


Figure 2. Flow chart of the computer program for simulation of the Smelting-Reduction process.

3. RESULTS AND DISCUSSION

Model calculations show that the most effective parameters influencing the consumption of materials and energy are PCR and PRD. While these quantities are strongly inter-related, PCR and the rate of injection of oxygen are nearly in proportion. PRD depends both on O_2/CO ratio and reforming of the combusted gas. In order to determine the interrelated effects of these parameter, a 100-ton reactor with specifications summerized in Table I is employed.

Table I Specifications of a Sample Double-Vessel Smelting-Reduction Process used for Calculations.

| Parameter | Value |
|----------------------------------|-----------------------|
| Area of molten metal pool | 30 m ² |
| Temperature of molten metal | 1723 °C |
| Carbon content of metallic melt | 3.5 Wt% |
| Density of molten metal | 7000Kg/m ³ |
| Heat capacity of metallic melt | 500 J/Kg°K |
| Density of gas | 0.5 Kg/m3 |
| Minimum diameter of droplets | 0.00005 m |
| Initial speed of droplets | 2 m/s |
| Rate of formation of droplets | 550 Kg/s |
| FeO content of slag | 5 percent |
| Productivity of the process | 40 ton/hr |
| Pre-reduction temperature | 1123 °K |
| Diameter of pre-reduction vessel | 6 m |

Figure 3 demonstrates the effect of PCR on PRD and the weight of coal that must be charged into the furnace. Small increases of up to 8 percent in PCR do not considerably influence the pre-reduction degree but sunstantially reduces the consumption of coal. Relative insensivity of PRD may be due to the

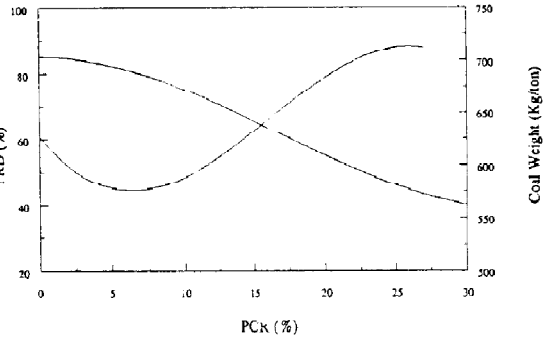


Figure 3. Effect of PCR on PRD and coal consumption in a double-vessel reactor without gas reformer.

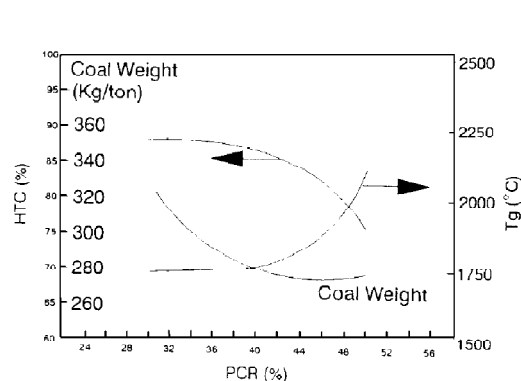


Figure 4. Effect of PCR on HTC, coal consumption and gas temperature in a double-vessel smelting-reduction system with gas reformer.

chemical reserve zones existing in the lower part of the pre-reduction shaft. The reduction in coal consumption is due to the large releases of the combustional heat.

Effect of PCR on HTC, T_g and coal weight in a combined smelting-reduction unit comprising of the maximum accessible natural-gas-reforming is represented in Figure 4. As is shown in the figure, the consumption of coal can be reduced to about 50 percent of the previous case by greatest utilization of the thermal energies and subsequent enhancements of PRD through reforming of the off-gas. This can lead the way to a suitable alternative for optimization of material and energy consumptions.

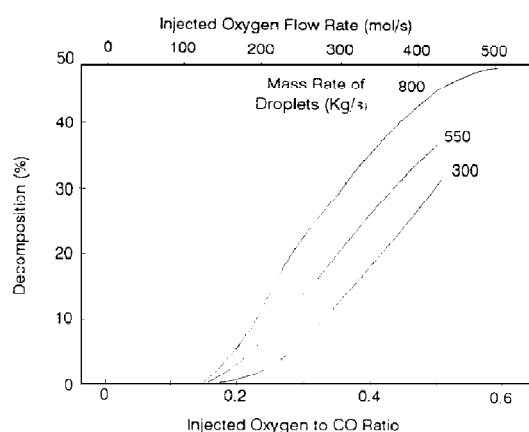


Figure 5. Effect of injection of O_2 and formation of liquid droplets on thermal decomposition of CO_2 .

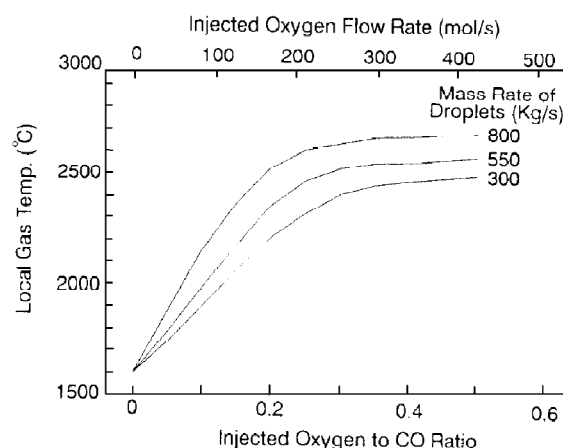


Figure 6. Effect of injection of O_2 and formation of liquid droplets on local gas temperature.

Model calculations show, however, a seizure in reduction of coal rate when PCR exceeds 40 percent. This is an unfavourable condition which lowers the efficiency of transfer of heat and increases the temperature of the exhausting gas (Figure 4). Under these conditions the destruction of refractory materials by melting and dissociation of CO_2 because of excessive heating can occur in the system (Figure 5).

Simulation results on the effect of PCR on the gas temperature is illustrated in Figure 6. As is shown in the figure, the gas temperature increases with the rate of injection of O_2 . Rate of formation of liquid droplets should also increase with the local gas temperature. The liquid droplets play an important role in formation of a

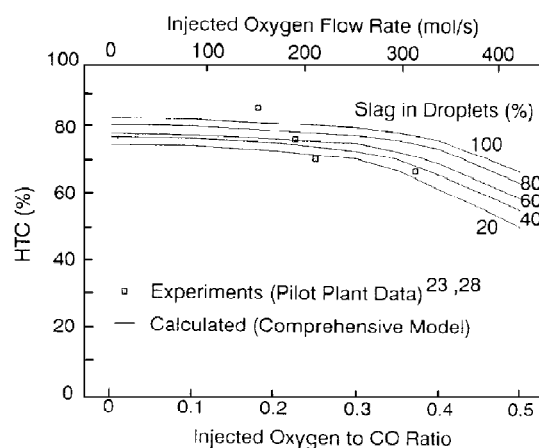


Figure 7. Effect of injection of O_2 and composition of droplets on efficiency of transfer of heat from gas to the melt.

thick layer of slag above the pool of liquid melt. This layer acts as an intermediate phase for transfer of heat from the hot gas to the liquid melt. It should be noted that efficiency of transfer of heat and temperature of gas both depend on production rate and the composition of the droplets (Figures 6 and 7).

A comparison is made in Figures 7 of the computed data with the experimental pilot results obtained by other investigators^{23,28}. Based on these data, a deep pool of slag collected on the top of the metallic bath can result in a higher droplet production rate, a lower slag FeO content and a better protection of the metallic melt from re-oxidation. This can help a lower S content, a more efficient energy consumption and a greater semi-steel production rate.

Increasing the surface area and the number of oxygen blowing sites improves the heating efficiency of the system (Figure 8) without excessive addition of gas temperature. This is achieved through enhancement of the number of liquid droplets that absorb heat from the gas. The extent and the number of blowing sites are represented by an empirical parameter P that affects on the heating efficiency by:

$$\eta = 100 - 90 \left(\frac{PCR}{100} \right)^{0.9} \frac{1}{P} \quad (18)$$

This equation clearly indicates that in order to achieve a required combustion ratio, the quantities of P and PCR can be appropriately controlled so that the heating efficiency would not be reduced.

4. CONCLUSIONS

A comprehensive computer model is developed for prediction of behavior of a combined bath-smelting

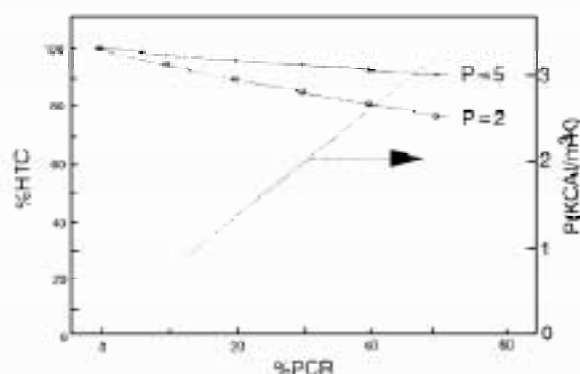


Figure 8. Effect of post combustion ratio and injection surface area on heating efficiency of the system.

pre-reduction units. Simultaneous transfer of heat from a post-combusted gas to iron or slag droplets suspended in the gas phase and serving as the medium which finally transfers heat to the melt is considered. The variation of temperature and composition of the CO₂ containing gas when mixed and reformed with alternative fuels and its effects on pre-reduction of the solid burden and the coal consumption rate are taken into account. Numerical calculations are carried out on the basis of thermodynamics, kinetics and transport phenomena equations in different sections of the system.

The program is capable to evaluate the following parameters:

- Pre-reduction degree
- Effect of post combustion and reforming of the off-gas on efficiency of transfer of heat
- Effect of post combustion and reforming of the off-gas on pre-reduction degree
- Effect of post combustion and reforming of the off-gas on coal consumption
- Effect of rate of formation and composition of liquid droplets on heat transfer efficiency and temperature and chemical decomposition of the gas
- Weights of coal, flux, ore, oxygen, natural gas, metallic product and slag
- Chemical composition of the liquid melt (%S, %C, %P, etc.)
- Temperature, composition and volume of the off-gas
- Efficiency of transfer of heat
- Over-all productivity of the smelting-reduction unit.

Several conclusions are obtained from application of the model to specific cases of general interest:

If reforming of the post combusted gas is not in order, excessive post combustion is not desirable.

With application of a natural gas reforming box, it is possible to obtain a PRD of 75 percent coupled with a post combustion ratio of up to 50 Percent and a minimum consumption of coal. The temperature of the exhausting gas would, however, be too high under these conditions.

For a post combustion ratio of up to 40 percent without reforming, the efficiency of transfer of heat decreases only slightly.

For post combustion ratios greater than 40 percent, the efficiency of transfer of heat decreases due to the greater heat loss and the lower proportion of heat that can be absorbed by the liquid phases.

A further increase in PCR without gas reforming results in a sharper decrease in obtainable PRD and a considerable reduction in HTC which causes a substantial increase in the rate of consumption of coal. The minimum consumption of coal and the

corresponding PCR both represent interesting base lines for designing an optimum combined smelting-reduction unit when reforming of the combusted gas is not to be practiced.

A highly increasing gas temperature is not desirable because it can cause (a) melting of refractory walls, (b) decomposition of CO₂ and (c) diminution of the heat transfer efficiency.

Reforming of the combusted off-gas together with increasing of the extent of blowing sites can improve the utilization of both thermal and chemical gas potentials and achievement of optimum operational conditions.

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