Dynamic Modeling of LD Converter Processes

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ABSTRACT

Because of the important role LD converters play in the production of high quality steel, various dynamic models have been attempted in the past by many researchers not only to understand the complex chemical reactions that take place in the converter process but also to assist the converter operation itself using computers. And yet no single dynamic model was found to be completely satisfactory because of the complexity involved with the process. The process indeed involves dynamic energy and mass balances at high temperatures accompanied by complex chemical reactions and transport phenomena in the molten state.

In the present study, a mathematical model describing the dynamic behavior of LD converter process has been developed. The dynamic model describes the time behavior of the temperature and the concentrations of chemical species in the hot metal bath and slag. The analysis was greatly facilitated by dividing the entire process into three zones according to the physical boundaries and reaction mechanisms. These three zones were hot metal (zone 1), slag (zone 2) and emulsion (zone 3) zones.

The removal rate of Si, C, Mn and P and the rate of Fe oxidation in the hot metal bath, and the change of composition in the slag were obtained as functions of time, operating conditions and kinetic parameters. The temperature behavior in the metal bath and the slag was also obtained by considering the heat transfer between the mixing and the slag zones and the heat generated from chemical reactions involving oxygen blowing.

To identify the unknown parameters in the equations and simulate the dynamic model, Hooke and Jeeves parttern search and Runge-Kutta integration algorithm were used. By testing and fitting the model with the data obtained from the operation of POSCO #2 steelmaking plant, the dynamic model was able to ·predict the characteristics of the main components in the LD converter. It was possible to predict the optimum CO gas recovery by computer simulation

1. Introduction

Nearly 30 years has passed since LD(Linz-Donawitz) converters (or basic oxygen furnace) went into operation and many dynamic models of LD processes have been proposed to improve the production of high quality steel[1].

The dynamic models are to describe the rate of change of bath temperature and slag compositions throughout the operation taking into account the variations of blowing conditions of oxygen. Although various dynamic models for the process have been suggested in the past, yet no dynamic model is found to be satisfactory because of very complex nature of reactions and transport phenomena taking place in the LD converter.   ·

In the present study, a dynamic model for the LD process is developed.   The dynamic model describes quantitatively time dependence of various components in the LD converter. It is used to evaluate the amount of carbon and temperature variations with oxygen blowing time and also to predict the recovering quantity of LDG (Linz-Donawitz gas, by-product gas). It also determines the end-point optimal concentration of carbon and bath temperature of the produced steel. The most important composition is the final carbon content in the molten iron through decarbonization and bath temperature which are influenced by complex chemical reactions (Si,Mn,P,Fe etc). In treating this complex process, the LD converter is divided into three zones according to the physical boundaries and reaction mechanisms. And then the dynamical balance equations of mass and energy are derived according to the reaction mechanisms involved. The parameter identification is then carried out. Since the oxidation of Si, Mn, P and Fe and reactions of slag components have influence on the composition behavior of C and bath temperature, the reaction mechanisms and dynamical equations for these components are individually developed. The flow pattern of oxygen also has very strong influence on the amount of carbon content and bath temperature.

Oxygen is supplied from two sources. One is the oxygen blown through the lance and the other is from the iron ore which is introduced to control the bath temperature. After the unknown parameters in the model are identified based on the plant data, the dynamic model is able to predict the characteristics of the main components in the LD converter. It is possible to predict the optimum CO gas recovery from the model as well.

2. Model Zones within LD Converter

Since it is very difficult to describe the complex microscopic dynamic behavior in the LD converter,

the dynamical analysis can be greatly facilitated if the entire process is divided into three zones according to the physical boundaries and reaction mechanisms as was done by Hwang et al.[2]
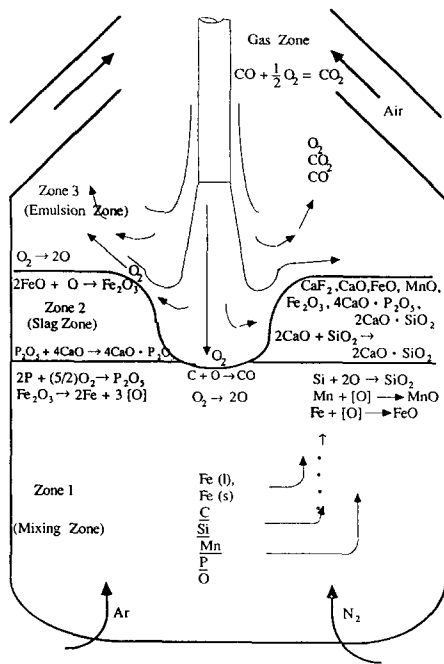

Figure 1. Schematic representation of oxidation reactions in the LD converter.

As shown in Fig.1., the first zone is hot metal(zone 1), the second zone slag and the third zone emulsion (zone 3). In zone 1, compositions in hot metal are fully mixed throughout the zone 1 by the oxygen which is blown at mach velocity from the lance and the inert gases (N_2, Ar) blown from the bottom. Thus it is nearly fully mixed concentration of components everywhere in this zone. Reactants in hot metal such as carbon, silicon, posphorous, manganeese react with oxygen at slag/metal and metal/gas interfaces. As a result, the oxide compounds except for decarbonization form slag. Iron ore which supplies a part of oxygen and plays a role of temperature control is sometimes introduced in the conveter during the operation. It dissociates into oxygen and Fe by direct reduction. Dissociated iron, scrap, and pig-iron in hot metal are partially melted into liquid during the operation.

In zone 2, the flux which is charged in the converter at the initial time reacts with oxide compounds as in zone 1. As a result of these reactions, slag is formed.[3,4] Silicon plays a very important role of not only in temperature control in the first part of the process because of large reactivity and enthalpy but also in the determination of the basicity for its complete oxidation. Thus knowing the initial silicon concentration, it is possible to calculate the exact amount of flux to be introduced. In this zone 2, a part of FeO and Fe_2O_3 are produced by oxygen and Fe. After the operation, some of slag is left to

protect the LD converter wall from damages.

The third zone (zone 3) is an emulsion zone consisting of iron particles containing carbon and impurities which are emulsified by the impact of oxygen from the lance against hot metal zone. CO and CO_2 gases of decarbonization contribute to the large apparent volume of this zone. In fact, it is possible to classify theoretically the slag zone and emulsion zone but it is very difficult in practice. Slopping due to some operating conditions such as strong oxide agents in scrap or oxygen blowing pattern can occur and have strong influence on the LD process. Since the reaction surface of iron particles is very large, direct oxidation in this zone increases the effect of decarbonization.

3. Dynamical Equations in Zones 1, 2 and 3

In the present study, we adopted the basic principle suggested by I Muchi[5,6], R.Weeks[7], and improved it to suit for for a real system. The mass balance equations are developed under the conditions that the process does not have slopping and the factors which are not amenable to theory are determined experimentally. In addition, the following assumptions are made:

a) The convective mass transfer of C, Si, Mn and P from the hot metal zone to other zones is negligible.
b) CO, O_2, and CO_2, are very close to ideal gases.
c) The main components are C, Si, Mn, P, and Fe in hot metal.
d) The main component of scrap introduced is Fe.
e) Fe_2O_3 is the main component of iron ore.
f) The influence on fume is neglected.
g) Lime has 100% CaO.

For Zone 1

The main reactants are C, Si, P, Mn etc. The solid particles such as C and P which are mixed in liquid iron at bath temperature react with oxygen gas. Therefore, reactions in the LD converter are typically heterogeneous.

To set up the dynamic mass balance for each component in this zone, it is necessary to consider the rate of change of the amount of each component due to chemical reaction. The dynamic mass balance of hot-metal is as follows:

$$\frac{d(W_{HM})}{dt} = \frac{(W^{\circ}_{HM})}{100} \times [(C_C^{*}(t)) - (X_{Mn}^{*}(t)) - (X_{Si}^{*}(t))$$
$$- (X_P^{*}(t))] + W_{pig\text{-}sol}(t) + W_{SCR\text{-}sol}(t)$$
$$- W_{FeO}(t) + W^{\circ}_{Fe_2O_3}(U(t)\text{-}U(t\text{-}t_0)) + W_{O_2}^{lance}(t) \quad (1)$$

where W°_{HM} is the weight of hot metal,Wpig-sol(t) and Wpig-sol(t) are weights of pig-iron and scrap which depend on time.

The calculation of the changing rate of the amount of pig-iron and scrap was accomplished by a operation pattern model obtained from the real operation. $W^{\circ}_{Fe_2O_3}(U(t)\text{-}U(t\text{-}t_0))$ expresses the input weight of iron ore which is assumed to melt and dissociate directly into O_2 and Fe as soon as it is

introduced into the LD converter.

To discribe the dynamic behavior of oxygen, the equation for oxygen blowing pattern which is made in the real operation is applied. Cc%(t), Xmn%(t), Xsi%(t), and Xp%(t) are the weight precent concentrations of carbon, manganese, silicon, and posphorous, respectively. The dynamic mass balance equation including those terms can be written as

$$\frac{d(W\,C_i)}{dt} = -R_i W - K_{1j} A_{1j} (C_i^1 - C_i^j) - F(C_i^1)$$
$$+ F(C_i^3) \quad (2)$$

where R_i = reaction rate equation of composition i
     i = composition of ith component in hot metal (C, Mn, P, Si)
     K_{ij} = mass transfer coefficient from zone 1 to zone j
     A_{1j} = interface area between zone 1 and j
     j = zone 2 or zone 3 (zones except for zone1)
     F = physical movement
     C_i = weight percent of ith component
     W = hot metal weight

According to the assumption (a), the term of convective mass transfer of reactants in the right hand side is neglected and F term is deleted because it is small in comparison with hot metal weight. Thus the equation 2 is simplified to

$$\frac{d(W\,C_i)}{dt} = -R_i W \quad (3)$$

Since there are heterogeneous reactions in zone 1, the reactions are divided into three steps; mass transfer of reactants to the phase boundary, interfacial chemical reaction, and mass transfer of reaction products away from the phase boundary. In the process of high temperatue above 1600K, it is generally agreed that the chemical reaction is much faster than the others and that refining reactions are effectively limited by mass transfer. Hence mass transfer is determined as a rate controlling step. Therefore, the rate equation is expressed by Fick's law.

The dynamic behavior of C depends on oxygen and bath temperature. O_2 gases out of the lance and Fe_2O_3(iron-ore) are delivered to the hot-metal zone(zone1). Dissociation of iron ore is a direct reaction given by

$$Fe_2O_3 = 2Fe + 3\,[O]$$
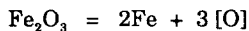
The most of its oxygen molecules react with C and impurities at its surface and the rest of them do in zone 3.

The reaction mechanism of carbon removal is the direct reaction of carbon in the hot metal surface with oxygen from the lance and the iron ore:

$$C + [O] \longrightarrow CO(g)$$
$$C + O_2 \longrightarrow CO_2(g)$$
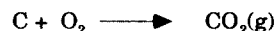
The following equation represents the behavior of C which is one of the main target compositions of LD process.

$$\frac{d(C\%)}{dt} = \frac{-1201}{1600} \cdot \frac{RK_O \rho_{HM}}{W_{HM}} \cdot \frac{P_T}{P_{CO} + 2P_{CO_2}}$$
$$\times \left[O\% - \frac{P_{CO}}{f_C \cdot C\% f_O K_{CO} G^2} \right] \quad (4)$$

where C% is the weight percent of carbon, W_{HM} is the hot-metel weight, RK_O is the reaction rate constant of decarbonization, ρ_{HM} is the density of hot-metal, P_T is the total pressure, P_{CO} and P_{CO_2} are partial pressures of CO and CO_2, f_C and f_O are activity coefficients of C and O_2, $K_{C,O}$ is the equilibrium constant of CO, and G is the inverse of hot metal ratio.

The typical oxidation mechanism of Mn is a direct reaction whose source is oxygen coming directly from the lance:[7]

$$Mn + O \longrightarrow MnO$$

And the total Mn behavior is described stoichiometrically. The controlling step for the rate equation of Mn is the diffusion of MnO at the inferface. The reaction rate is expressed as follows:

$$\frac{d(X_{Mn}\%)}{dt} = \frac{RK_{MnO} \cdot \rho_{s1}}{W_{HM}^0 \cdot W_{s1}} \left[\frac{5493\,K_{MnO} \cdot Z \cdot G^2}{f_{MnO}} \right.$$
$$\left. \times f_{Mn}(Mn\% - X_{Mn}\%) f_0 \cdot O\% - W_{HM}^0 \cdot X_{Mn}\% \right] \quad (5)$$

Where Xmn% is the weight precent of Mn, and ρ_{s1} and W_{s1} are the slag density and the slag weight. Z represents the total number of slag moles. Mn% is the initial weight percent concentration of Mn.

The reaction mechanism of P is a direct reaction with O_2 from the lance and iron ore:

$$2P + (5/2)O_2 \longrightarrow P_2O_5$$

The most of P_2O_5 in the zone 1 reacts with CaO sequentialy to produce $CaO \cdot P_2O_5$ in the zone 2 (slag zone) and the rest makes reversible reaction to return P to the hot metal zone. The dynamic behavior of P shows the same pattern as that of Mn. The equation is as follows:

$$\frac{d(X_P\%)}{dt} = 2RK_{P_2O_5} \rho_{s1} \left[\frac{10^Y}{W_{HM}} (P_o\% - Xp\%) - \frac{X_P\%}{2 \cdot W_{s1}} \right]$$
$$RK_{P_2O_5} = D_{P_2O_5} A\,\rho_{s1} / \Delta\delta \quad (6)$$

where Po% is the initial weight percent concentration of P, Y is the ratio of distribution of P, $D_{p_2o_5}$ is the diffusion coefficient, A is the reaction interface area, and $\Delta\delta$ is the boundary film thickness.

Silicon plays a important role in the LD process because its complete oxidation is possible to calculate the bascity of the process to determine the amount of flux. Chemical reaction is as follows:

$$Si(l) + O_2(g) \longrightarrow SiO_2(s)$$

The following equation expresses the dynamic characteristics of silicon in the zone 1:

$$\frac{d(X_{si}\%)}{dt} = \frac{RK_{si}\,\rho_{HM}}{W_{HM}}(Si_i\% - X_{si}\%) \tag{7}$$

where $X_{Si}\%$ is the weight precent concentration of Si, Si% is the initial concentration of Si, and RKsi is the rate constant of Si. The reaction control step of oxidation is the diffusion of Si.

For Zone 2

This zone is made of flux such as CaO, dolomite, and oxide compounds which are the reaction products from zone 1. In this zone, there are main reactions of P_2O_5 with CaO, SiO_2 with CaO, FeO with oxygen, and a reversible reaction of MnO[3,4,]

The suggested oxidation reaction of P is as follows:

$$P_2O_5 + m\,CaO \rightleftarrows m\,CaO\cdot P_2O_5 \quad (m=4)$$

The reaction mechanism for silicon oxide is similar to that of P_2O_5. The reaction of CaO and SiO_2 makes a stable silicon compound. The suggested reaction is as follows:

$$SiO_2 + nCaO \longrightarrow nCaO\cdot SiO_2 \quad (n=2)$$

The effect of Fe_2O_3 and Mg is neglected. Hence the dynamic behavior of each component in the zone 2 is closely connected with that of each component in the zone 1 because the oxide compounds of the impurities become a large part of the slag in the zone 2. The dynamical equations for zone 2 is as follows:

$$\frac{d(W_{sl})}{dt} = \frac{W^\circ_{HM}}{100}(X_P\%(t) + X_{Mn}\%(t) + X_{Si}\%(t)) +$$
$$W_{CaO}(t) + W_{FeO}(t) \tag{8}$$

where W°_{HM} is the initial hot metal weight, $Wc_ao(t)$ is the weight of CaO, and $W_{FeO}(t)$ is the weight of FeO. In equation (8), it is assumed that the reaction products of impurities at the zone 1 become slag entirely. The oxygen which reacts with some of iron in hot metal makes FeO and Fe_2O_3 which are a part of oxygen sources. The reaction is as follows:

$$Fe + O \rightleftarrows FeO \text{ (slag)}$$
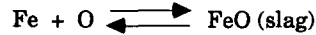
The change of W_{FeO} with time is calculated by the opreration model deduced from experiences which uses stoicheometry of Fe and O_2. And then the total amount of Fe in the slag is determined. It is also assumed that the amount of Fe_2O_3 in the slag is neglected because the ratio of Fe_2O_3 to FeO is relatively small and it is very difficult to describe the mechanism. The melting rate of CaO (flux) is expressed as follows:

$$\frac{d(X_{CaO})}{dt} = \frac{3\alpha}{t_A} \times (t/t_A - 1)^2 \tag{9}$$

where X_{CaO} is the weight change of CaO, t_A and α are factors in the real operation.

For Zone 3

Since zone 3 is a very complex emulsion zone where slag, gases, fume and a part of compositions of hot metal are dynamically mixed, it is very difficult to describe quantitatively the dynamic behavior of reactants. So it is considered only C as a reactant because the other impurities are assumed to have little influence on the process. The mechanism of decarbonization is assumed to be the same as that of the zone 1. Therefore it is possible to describe quantitatively the behavior as combining the terms of reaction rate constants of zone 1 and zone 3. It increases the total reaction area according to the equation:

$$RK_i = \frac{D_i(A_1 + A_3)}{\Delta\delta} = \frac{D_iA}{\Delta\delta} \tag{10}$$

where RK_i is the reaction rate constant of i component, A1 and A3 are reaction interface areas between zone 1 and oxygen and between zone 2 and oxygen, D_i is the diffusion coefficient and $\Delta\delta$ is the film thickness. Gases and fumes formed from this zone get out of the pipe set above the converter. In the present study, the effect of fume is neglected. LDG, the product gas is used as a valuable energy source.

Assumptions made for the energy balance are
  (1) For temperatures, the three zones are treated as one.
  (2) Temperature in the converter is equal to that of hot metal.

The equations for energy balance is as follows:

$$\frac{d}{dt}(C_{P_{HM}} W_{HM} T_{HM}) = -\sum_1^{M_i}[(\Delta H_i + \frac{}{M_i} C_{P_i}(T_{HM} - T_o)]$$
$$\times\ W_{HM}(-R_i)/100] - \{\Delta H_{Fe\text{-}FeO}\,55.8\,/\,M_{FeO} + C_{P_{FeO}}$$
$$(T_{HM} - T_o)]\times W_{FeO}(t) - [\Delta H_{Fe_2O_3\text{-}Fe}\,111.7\,/\,M_{Fe} -$$
$$C_{P_{Fe2O3}}(T_{HM} - T_o)]\times W_{ore}(t) + Q \tag{11}$$

where C_{Pi} is the specific heat capacity of component i, ΔH is the heat of reaction, M is the molecular weight, l is the product, and i is the reactant. T_{HM} is the bath temperature (hot metal temperature). T_o is the standard state temperature and Q is the heat loss.

4. Parameter Identification

Parameters estimated by the optimization technique are four reaction constants for C, Mn, P, and Si consisting of a diffusion coefficient, a reaction interface area and a film thickness Mn. The other factors and data are collected from the operation data and reference books.[8,9]

The parameters are estimated by an optimization method using Hook and Jeeves pattern search which is appropriate for systems of the nonlinear differential equations.[10] It is indeed possible to approach the nonlinear differential system whose objective function for parameter estimation cannot be expressed as equations but as numerical values. Therefore although the pattern search method is slower and less elegant than a gradient method, it is very useful in optimum parameter estimation.

The flow sheet of the dynamic simulation is given in Figure 2. In Figure 2, the initial parameter values are 48 for C, 0.018 for P, 0.2948 for Mn, and 71 for Si. The step length for optimum pattern search was 0.0025 at first. Unit sampling data for C, Mn, P, and Si are weight percents of compositions. The objective function is the sum of squares of errors between sampling data and calculated value:

squares of errors between sampling data and calculated values:

$$f_{obj} = \Sigma e^2 = \sum_{t=t_i}^{t_e} \sum_{i=1}^{L} (C_i^{exp} - C_i^{cal})^2 \qquad (12)$$

where f_{obj} is the objective function, t_i is the initial sampling time, t_e is the final sampling time, and i is the reactant, and the weighting factor is 1. The sampling data are obtained from Pohang Steel Works, POSCO #2 steel-making unit.

Equation for Hooke and Jeeves method is given by

$$(RK^0_{BC} + D_1) = (RK^0_{BC} + d_1, RK^0_{BP}, RK^0_{BMn}, RK^0_{BSi}) \qquad (13)$$

where RK^0_{BC} is the initial reaction rate constant of C, D and d are the step lengths, RK^0_{BP}, RK^0_{BP}, RK^0_{BMn}, and RK^0_{BSi} are the initial rate constants of P, Mn, and Si, respectively.

5. Dynamical Behaviors of Components in the LD Converter

There are seven main differential equations and other operation related equations in the dynamic model. Because of the nonlinearty of the equations, the solution was obtained by the fourth-order Runge-Kutta method suggested by Abramowitz Stegun, Gear, and others.

The steps for numerical solution are the following:

$$K^i_1 = dt\, f'(t_m, y_m)$$
$$K^i_2 = dt\, f'(t_m + h/2, C^i_m + K^i_1/2)$$
$$K^i_3 = dt\, f'(t_m + h/2, C^i_m + K^i_2/2)$$
$$K^i_4 = dt\, f'(t_m + h, C^i_m + K^i_3)$$
$$C^i_{m+1} = C^i_m + 1/6\,(K^i_1 + 2K^i_2 + 2K^i_3 + K^i_4)$$

where i represents a composition, C the weight percent concentration of each component.

The present dynamic model consisting of seven differential equations for the computer solution represents the total hot-metal balance, the energy balance and the composition mass balance. It was possible to calculate all the equations at the same step size for tracing out the concentrations of components and bath temperature at the same time. Step size is 1 minute and the computer used is IBM-PS/2 (Series 386 & model 70). The program is written in C-language.

The solution of the dynamic model equations is compared to sampling data obtained from real LD process. The initial values of parameter of C, P, Mn and Si are 48, 0.018, 0.2948 and 71, respectively and the finial estimated values are 48.0215, 0.004997, 0.4761 and 71.194.

Figure 3 shows the result of dynamic behavior of C which is the most important key component to be eliminated in LD process. From the result, it is seen that the theoretical dynamic behavior of C predicts very well the real plant data. At first period(step) of operation, decarbonization proceeds slowly because there is high concentration of high reactive compositions such as Si and Mn which are oxidized faster than C.
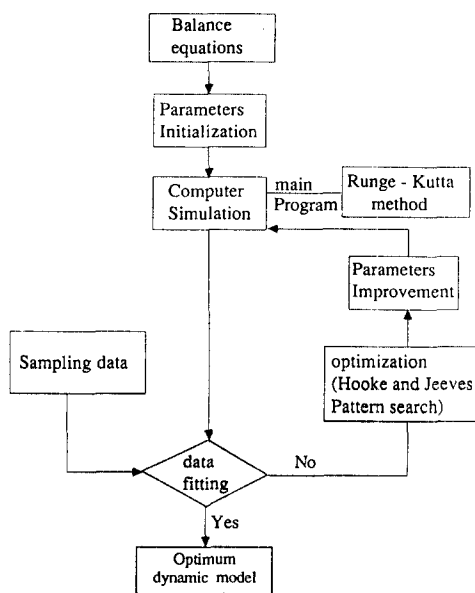

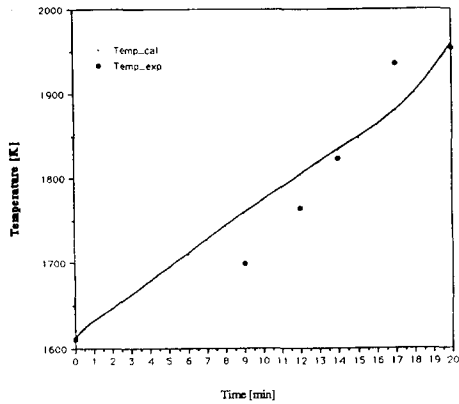Figure 2. Dynamic simulation flow chart for the LD process.

Fig. 3 Comparison of the experimental results with the theoretical ones for the rate of change of carbon at 80% HMR(hot metal ratio).

Therefore the distribution ratio of oxygen to C is relatively small. It is thought to be the reason why carbon removal rate is slow. With the oxygen blowing time, carbon removal rate is getting larger and at the half time the rate becomes maximum because Si is already removed within six mininutes (see Fig. 4) and other reactants except for C scarcely participate in oxidation at midst of operation. It can be also concluded that the reaction mechanism is governed by direct reactions. The behavior of P and Mn shows the good results in the begining of the process.

After the half time of the LD process, the amounts of the oxide compounds differed from the real data.
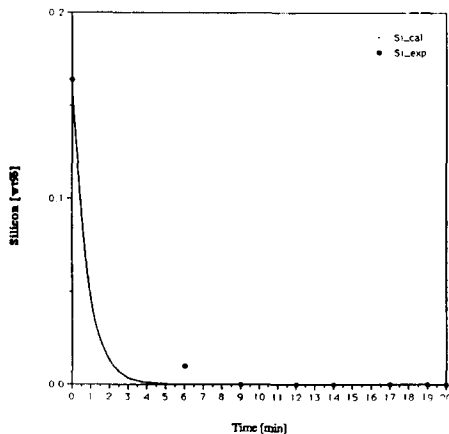

Figure 4. Comparison of the experimental results with the theoretical ones for the rate of Si change at 80% HMR

The behavior of bath temperature for the process highly depends on the nature of chemical reactions in the molten steel, especially carbon and silicon. Figure 5 shows the result of the simulation and the real opreating data. In figure 5, it is seen that the temperature behavior by simulation is somewhat
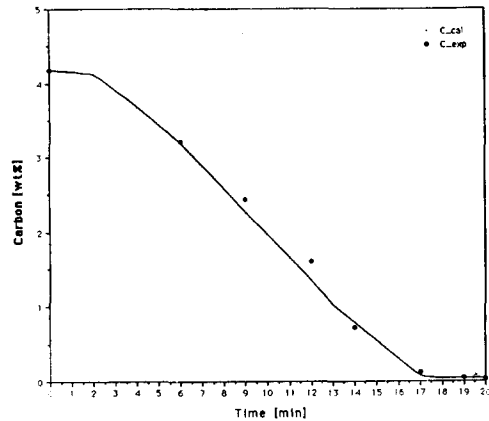

Figure 5. Comparison of the experimental results with the theoretical ones for the rate of temperature change at 80% HMR(hot metal ratio).

different from the real data. As oxygen blowing time approaches the end point, it is seen that the real temperature is slightly higher than that of the simulation. It means that as P and Mn which are released from oxidation react with FeO. This exothermic reaction causes   the temperature increase.

As a result of the dynamic oxygen simulation for the LD process, the amount of decarbonization is calculated to predict carbon monoxide and carbon dioxide wihich will be uscd as another energy source. Other representative gases which are produced during the LD operation are oxygen and nitrogen originally contained in the air which is introduced through the inlet pipe during blowing time, argon and nitrogen which facilitates complete mixing of the hot metal by bottom blowing, and CO, CO_2 gases produced by decarbonization reaction.

Based on the present study, we can develop the prediction method of an LDG holder level. Indeed the LDG balance and holder level are predicted by computer simulation with the bottom flow rate pattern which is determined by the present study. This method enhances the accuracy of the instantaneosly changing holder level by calculating gas generation per unit time. It will eventually contribute to the efficient energy distribution.

6. Conclusion

Concerning the oxidation of molten steel taking place in the various refining processes, a simplified mathematical model has been developed. There are compex reactions taking place in the LD process and some of operating conditions are difficult to describe exactly. In the present study, we have shown that the developed model can describe the dynamic behavior which agrees reasonably well with the operation data. On the other hand further research for P and Mn is required. The model developed in the present study can also be applied to solving a problem of optimal control of the process.

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