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Applicability of mass action law to sulphur distribution between slag melts and liquid iron

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Abstract: According to the mass action law and the coexistence theory of slag structure, the calculating models of mass action concentration for CaO-MgO-FeO-Fe_2O_3-SiO_2, CaO-MgO-MnO-FeO-Fe_2O_3-P_2O_5-SiO_2 and CaO-MgO-MnO-FeO-Fe_2O_3-Al_2O_3-P_2O_5-SiO_2 slag melts are formulated and sulphur distribution between the slag melts and liquid iron is treated. It is found that CaO, MnO and FeO promote desulphurization, while MgO is detrimental to desulphurization. In addition, the sulphur distribution coefficients between the slag melts and liquid iron are presented.

Key words: mass action law; coexistence theory of slag structure; activity; mass action concentration

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The sulphur distribution between CaO-MgO-FeO-Fe_2O_3-SiO_2 slag melt and liquid iron has been discussed [1], and the sulphur distribution coefficient

$$L_S = \frac{8(K_{CaS}N_{CaO} + K_{FeS}N_{FeO} + K_{MgS}N_{MgO})\sum n}{[O\%]},$$

$$MgO(s) + [S] = MgS_{(S)} + [O]$$

and

$$\Delta G^\circ = 199752 - 31.527T \ \text{(J/mol)}$$

have been used to evaluate K_{MgS} [2]. It seems theoretically reasonable to do so, because other researchers have obtained similar information about the desulphurization capability of MgO [3,4], *i.e.*, MgO has certain desulphurization capability, though it is very little. However, after treating a lot of equilibrium data about sulphur distribution between multicomponent slag melts and liquid iron, it was found that in the majority cases K_{MgS} are negative values. The objective of this paper is just to introduce the results of such treatment. In addition, checking whether the mass action law and the coexistence theory of slag structure are applicable to the sulphur distribution between multicomponent (over 5 components) and liquid iron is also an important question to be answered.

1 Sulphur distribution between CaO-MgO-FeO-Fe_2O_3-SiO_2 slag melt and liquid iron

According to the phase diagrams [5], there are Fe_2O_3, SiO_2, $CaFe_2O_4$, $Ca_2Fe_2O_5$, $MgFe_2O_4$, Fe_3O_4, $CaSiO_3$, Ca_2SiO_4, Ca_3SiO_5, $MgSiO_3$, Mg_2SiO_4, Fe_2SiO_4, $CaMgSiO_4$, $CaO{\cdot}MgO{\cdot}2SiO_2$, $2CaO{\cdot}MgO{\cdot}2SiO_2$ and $3CaO{\cdot}MgO{\cdot}2SiO_2$ formed in this slag system. Hence, based on the coexistence theory of slag structure [6], the structural units of the slag melt are Ca^{2+}, Mg^{2+}, Fe^{2+}, O^{2-}, S^{2-} simple ions as well as Fe_2O_3, SiO_2, $CaFe_2O_4$, $Ca_2Fe_2O_5$, $MgFe_2O_4$, Fe_3O_4, $CaSiO_3$, Ca_2SiO_4, Ca_3SiO_5, $MgSiO_3$, Mg_2SiO_4, Fe_2SiO_4, $CaMgSiO_4$, $CaO{\cdot}MgO{\cdot}2SiO_2$, $2CaO{\cdot}MgO{\cdot}2SiO_2$ and $3CaO{\cdot}MgO{\cdot}2SiO_2$ molecules.

Assuming the composition of the melt as

$b_1 = \sum n_{CaO}$, $b_2 = \sum n_{MgO}$, $b_3 = \sum n_{FeO}$, $a_1 = \sum n_{Fe_2O_3}$, $a_2 = \sum n_{SiO_2}$;

the equilibrium amount of every structural unit (in mol) expressed by the composition as

$x_1 = n_{CaO}$, $x_2 = n_{MgO}$, $x_3 = n_{FeO}$, $y_1 = n_{Fe_2O_3}$,

$y_2 = n_{SiO_2}$, $z_1 = n_{CaFe_2O_4}$, $z_2 = n_{Ca_2Fe_2O_5}$, $z_3 = n_{MgFe_2O_4}$,

$z_4 = n_{Fe_3O_4}$, $z_5 = n_{CaSiO_3}$, $z_6 = n_{Ca_2SiO_4}$, $z_7 = n_{Ca_3SiO_5}$,

$z_8 = n_{MgSiO_3}$, $z_9 = n_{Mg_2SiO_4}$, $z_{10} = n_{Fe_2SiO_4}$, $z_{11} = n_{CaMgSiO_4}$,

$z_{12} = n_{CaO\cdot MgO\cdot 2SiO_2}$, $z_{13} = n_{2CaO\cdot MgO\cdot 2SiO_2}$,

$z_{14} = n_{3CaO\cdot MgO\cdot 2SiO_2}$;

the mass action concentration of every structural unit after normalization as

$N_1 = N_{CaO}$, $N_2 = N_{MgO}$, $N_3 = N_{FeO}$, $N_4 = N_{Fe_2O_3}$,

$N_5 = N_{SiO_2}$, $N_6 = N_{CaFe_2O_4}$, $N_7 = N_{Ca_2Fe_2O_5}$,

$N_8 = N_{MgFe_2O_4}$, $N_9 = N_{Fe_3O_4}$, $N_{10} = N_{CaSiO_3}$,

$N_{11} = N_{Ca_2SiO_4}$, $N_{12} = N_{Ca_3SiO_5}$, $N_{13} = N_{MgSiO_3}$,

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$N_{14} = N_{Mg_2SiO_4}$, $N_{15} = N_{Fe_2SiO_4}$, $N_{16} = N_{CaMgSiO_4}$,

$N_{17} = N_{CaO\cdot MgO\cdot 2SiO_2}$, $N_{18} = N_{2CaO\cdot MgO\cdot 2SiO_2}$,

$N_{19} = N_{3CaO\cdot MgO\cdot 2SiO_2}$,

$\sum n$ = the sum of the amounts of ions and molecules in equilibrium (in mol). Then in the light of the mass action law, it gives as the following.

Chemical equilibria:

$(Ca^{2+} + O^{2-})_{(s)} + Fe_2O_{3(s)} = CaFe_2O_{4(s)}$,

$$K_1 = \frac{N_6}{N_1 N_4},\ z_1 = 2K_1 \frac{x_1 y_1}{\sum n} \tag{1}$$

$\Delta G^\circ = -29726 - 4.815\ T$ (J/mol), 973-1489 K [7];

$2(Ca^{2+} + O^{2-})_{(s)} + Fe_2O_{3(s)} = Ca_2Fe_2O_{5(s)}$,

$$K_2 = \frac{N_7}{N_1^2 N_4},\ z_2 = 4K_2 \frac{x_1^2 y_1}{(\sum n)^2} \tag{2}$$

$\Delta G^\circ = -53172-2.512\ T$ (J/mol), 973-1723 K [7]

$(Mg^{2+} + O^{2-})_{(s)} + Fe_2O_{3(s)} = MgFe_2O_{4(s)}$,

$$K_3 = \frac{N_8}{N_2 N_4},\quad z_3 = 2K_3 \frac{x_2 y_1}{\sum n} \tag{3}$$

$\Delta G^\circ = -19259 - 2.0934\ T$ (J/mol), 973-1673 K [7];

$(Fe^{2+} + O^{2-}) + Fe_2O_{3(s)} = Fe_3O_{4(s)}$,

$$K_4 = \frac{N_9}{N_3 N_4},\ z_4 = 2K_4 \frac{x_3 y_1}{\sum n} \tag{4}$$

$\Delta G^\circ = -45845.5 + 10.635\ T$ (J/mol), 1644-1870 K [6];

$(Ca^{2+} + O^{2-}) + (SiO_2) = (CaSiO_3)$,

$$K_5 = \frac{N_{10}}{N_1 N_5},\quad z_5 = 2K_5 \frac{x_1 y_2}{\sum n} \tag{5}$$

$\Delta G^\circ = -81416 - 10.498\ T$ (J/mol) [6];

$2(Ca^{2+} + O^{2-}) + (SiO_2) = (Ca_2SiO_4)$,

$$K_6 = \frac{N_{11}}{N_1^2 N_5},\ z_6 = 4K_6 \frac{x_1^2 y_2}{(\sum n)^2} \tag{6}$$

$\Delta G^\circ = -160431 + 4.106\ T$ (J/mol) [6];

$3(Ca^{2+} + O^{2-}) + (SiO_2) = (Ca_3SiO_5)$,

$$K_7 = \frac{N_{12}}{N_1^3 N_5},\quad z_7 = 8K_7 \frac{x_1^3 y_2}{(\sum n)^3} \tag{7}$$

$\Delta G^\circ = -93366 - 23.027\ T$ (J/mol) [8];

$(Mg^{2+} + O^{2-})_{(s)} + SiO_{2(s)} = MgSiO_{3(s)}$,

$$K_8 = \frac{N_{13}}{N_2 N_5},\ z_8 = 2K_8 \frac{x_2 y_2}{\sum n} \tag{8}$$

$\Delta G^\circ = -36425 + 1.675\ T$ (J/mol) [9];

$2(Mg^{2+} + O^{2-})_{(s)} + SiO_{2(s)} = Mg_2SiO_{4(s)}$,

$$K_9 = \frac{N_{14}}{N_2^2 N_5},\ z_9 = 4K_9 \frac{x_2^2 y_2}{(\sum n)^2} \tag{9}$$

$\Delta G^\circ = -63220 + 1.884\ T$ (J/mol) [9];

$2(Fe^{2+} + O^{2-}) + (SiO_2) = (Fe_2SiO_4)$,

$$K_{10} = \frac{N_{15}}{N_3^2 N_5},\ z_{10} = 4K_{10} \frac{x_3^2 y_2}{(\sum n)^2} \tag{10}$$

$\Delta G^\circ = -28596 + 3.349\ T$ (J/mol), 1808-1986 K [10];

$(Ca^{2+} + O^{2-})_{(s)} + (Mg^{2+} + O^{2-})_{(s)} + SiO_{2(s)} = CaMgSiO_{4(s)}$,

$$K_{11} = \frac{N_{16}}{N_1 N_2 N_5},\ z_{11} = 4K_{11} \frac{x_1 x_2 y_2}{(\sum n)^2} \tag{11}$$

$\Delta G^\circ = -124766.6 + 3.768\ T$ (J/mol), 298-1473 K [7];

$(Ca^{2+} + O^{2-}) + (Mg^{2+} + O^{2-}) + 2(SiO_2) = (CaMgSi_2O_6)$,

$$K_{12} = \frac{N_{17}}{N_1 N_2 N_5^2},\ z_{12} = 4K_{12} \frac{x_1 x_2 y_2^2}{(\sum n)^3} \tag{12}$$

$\Delta G^\circ = -80387 - 51.916\ T$ (J/mol) [11];

$2(Ca^{2+} + O^{2-}) + (Mg^{2+} + O^{2-}) + 2(SiO_2) = (Ca_2MgSi_2O_7)$,

$$K_{13} = \frac{N_{18}}{N_1^2 N_2 N_5^2},\ z_{13} = 8K_{13} \frac{x_1^2 x_2 y_2^2}{(\sum n)^4} \tag{13}$$

$\Delta G^\circ = -73688 - 63.639\ T$ (J/mol) [11];

$3(Ca^{2+} + O^{2-}) + (Mg^{2+} + O^{2-}) + 2(SiO_2) = (Ca_3MgSi_2O_8)$,

$$K_{14} = \frac{N_{19}}{N_1^3 N_2 N_5^2},\ z_{14} = 16K_{14} \frac{x_1^3 x_2 y_2^2}{(\sum n)^5} \tag{14}$$

$\Delta G^\circ = -315469 + 24.786\ T$ (J/mol) [12].

Mass balance:

$$b_1 = x_1 + z_1 + 2z_2 + z_5 + 2z_6 + 3z_7 + z_{11} + z_{12} + 2z_{13} + 3z_{14} \tag{15}$$

$$b_2 = x_2 + z_3 + z_8 + 2z_9 + z_{11} + z_{12} + z_{13} + z_{14} \tag{16}$$

$$b_3 = x_3 + z_4 + 2z_{10} \tag{17}$$

$$a_1 = y_1 + z_1 + z_2 + z_3 + z_4 \tag{18}$$

$$a_2 = y_2 + z_5 + z_6 + z_7 + z_8 + z_9 + z_{10} + z_{11} + 2z_{12} + 2z_{13} + 2z_{14} \tag{19}$$

$$\sum n = 2\sum_{i=1}^{3} x_i + \sum_{j=1}^{2} y_j + \sum_{k=1}^{14} z_k \tag{20}$$

The mass action concentration of every structural unit can be respectively expressed as

$$N_i = \frac{2x_i}{\sum n} \tag{21}$$

where the subscript i indicates CaO, MgO, FeO *etc.*

$$N_j = \frac{z_j}{\sum n} \tag{22}$$

where the subscript j indicates Fe_2O_3, SiO_2, silicates *etc.*

The above-mentioned equations (1)-(22) are the calculating model of mass action concentrations for the slag melt. The sulphur distribution reactions between the slag melt and liquid iron are illustrated by the following equations:

$$(Ca^{2+} + O^{2-}) + [S] = (Ca^{2+} + S^{2-}) + [O],$$

$$K_{CaS} = \frac{N_{CaS}N_{[O]}}{N_{CaO}N_{[S]}} = \frac{\frac{2(S)_{CaS}}{32\sum n} \cdot \frac{[O]}{16\times 1.7905}}{\frac{2x_1}{\sum n} \cdot \frac{[S]}{32\times 1.7905}} = \frac{(S)_{CaS}[O]}{8N_{CaO}[S]\sum n},$$

$$L_{CaS} = 8K_{CaS}N_{CaO}\frac{\sum n}{[O]} \tag{23}$$

Similarly,

$$(Mg^{2+} + O^{2-}) + [S] = (Mg^{2+} + S^{2-}) + [O],$$

$$L_{MgS} = 8K_{MgS}N_{MgO}\frac{\sum n}{[O]} \tag{24}$$

$$(Fe^{2+} + O^{2-}) + [S] = (Fe^{2+} + S^{2-}) + [O],$$

$$L_{FeS} = 8K_{FeS}N_{FeO}\frac{\sum n}{[O]} \tag{25}$$

Hence, the sulphur distribution coefficient between the slag melt and liquid iron is as follows:

$$L_S = \frac{8(K_{CaS}N_{CaO} + K_{MgS}N_{MgO} + K_{FeS}N_{FeO})\sum n}{[O]} \tag{26}$$

Transforming equation (26) into the following equation:

$$\frac{L_S[O]}{8\sum n\, N_{MgO}} = K_{MgS} + K_{CaS}N_{CaO} + K_{FeS}N_{FeO} \tag{26a}$$

and putting

$$Y = \frac{L_S[O]}{8\sum n\, N_{MgO}},\quad a = K_{MgS},\quad b_1 = K_{CaS},\quad X_1 = N_{CaO},$$

$$b_2 = K_{FeS},\quad X_2 = N_{FeO},$$

then equation (26a) changes to the following regression equation of two independent variables:

$$Y = a + b_1X_1 + b_2X_2 .$$

Using equilibrium sulphur distribution data between the slag melt and liquid iron from reference [13] as well as equations (1)-(22), the mass action concentration of the slag melt at different temperatures was calculated, then equation (26a) was used to regress the equilibrium constants of desulphurization for the slag melt as

$K_{CaS} = 0.060687$, $K_{FeS} = 0.049717$, $K_{MgS} = -0.02268$,

$R = 0.95068$, $F = 361.678$.

Thus, the coefficient of sulphur distribution for the slag melt and liquid iron can be expressed by the following equation:

$$L_S = [8(0.060687N_{CaO} + 0.049717N_{FeO} - 0.02268N_{MgO})\sum n]/[O\%].$$

The calculated results are shown in **Figure 1**. It can be seen from the figure that agreement between the calculated and measured values is good, and testified that the aforementioned calculating model can reflect the sulphur distribution characteristics between the slag melt and liquid iron. However, it should be pointed out that K_{MgS} is negative.

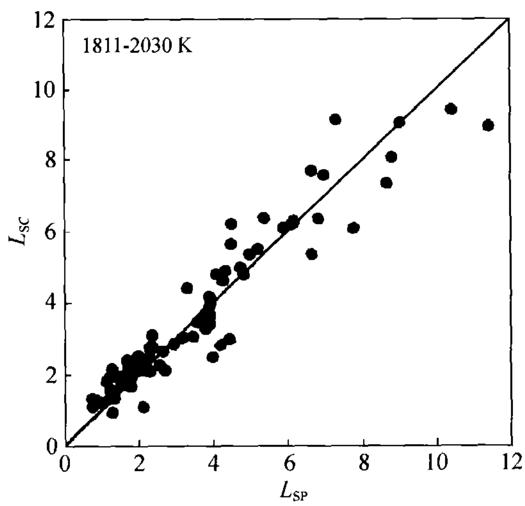

Figure 1 Comparison of the calculated L_{SC} values with the observed L_{SP} values at temperatures of 1811-2030 K.

2 Sulphur distribution between CaO-MgO-MnO-FeO-Fe₂O₃-P₂O₅-SiO₂ slag melt and liquid iron

In comparison with CaO-MgO-FeO-Fe_2O_3-SiO_2 slag system, as well as according to the phase diagrams [5] and the coexistence theory of slag structure [6], the additional structural units of the slag melt are Mn^{2+}, $MnFe_2O_4$, $MnSiO_3$, Mn_2SiO_4, $2CaO\cdot P_2O_5$, $3CaO\cdot P_2O_5$, $4CaO\cdot P_2O_5$, $2MgO\cdot P_2O_5$, $3MgO\cdot P_2O_5$, $3MnO\cdot P_2O_5$, $3FeO\cdot P_2O_5$ and $4FeO\cdot P_2O_5$.

Assuming the composition of the melt as

$$b_1 = \sum n_{CaO},\ b_2 = \sum n_{MgO},\ b_3 = \sum n_{MnO},\ b_4 = \sum n_{FeO}$$

$a_1 = \sum n_{Fe_2O_3}$, $a_2 = \sum n_{P_2O_5}$, $a_3 = \sum n_{SiO_2}$;

the equilibrium amount of every structural unit (in mol) expressed by the composition of the melt as

$x_1 = n_{CaO}$, $x_2 = n_{MgO}$, $x_3 = n_{MnO}$, $x_4 = n_{FeO}$, $y_1 = n_{Fe_2O_3}$,

$y_2 = n_{P_2O_5}$, $y_3 = n_{SiO_2}$, $z_1 = n_{CaFe_2O_4}$, $z_2 = n_{Ca_2Fe_2O_5}$,

$z_3 = n_{MgFe_2O_4}$, $z_4 = n_{MnFe_2O_4}$, $z_5 = n_{Fe_3O_4}$, $z_6 = n_{2CaO\cdot P_2O_5}$,

$z_7 = n_{3CaO\cdot P_2O_5}$, $z_8 = n_{4CaO\cdot P_2O_5}$, $z_9 = n_{2MgO\cdot P_2O_5}$,

$z_{10} = n_{3MgO\cdot P_2O_5}$, $z_{11} = n_{3MnO\cdot P_2O_5}$, $z_{12} = n_{3FeO\cdot P_2O_5}$,

$z_{13} = n_{4FeO\cdot P_2O_5}$, $z_{14} = n_{CaSiO_3}$, $z_{15} = n_{Ca_2SiO_4}$, $z_{16} = n_{Ca_3SiO_5}$,

$z_{17} = n_{MgSiO_3}$, $z_{18} = n_{Mg_2SiO_4}$, $z_{19} = n_{MnSiO_3}$, $z_{20} = n_{Mn_2SiO_4}$,

$z_{21} = n_{Fe_2SiO_4}$, $z_{22} = n_{CaMgSiO_4}$, $z_{23} = n_{CaO\cdot MgO\cdot 2SiO_2}$,

$z_{24} = n_{2CaO\cdot MgO\cdot 2SiO_2}$, $z_{25} = n_{3CaO\cdot MgO\cdot 2SiO_2}$;

the mass action concentration of every structural unit after normalization as

$N_1 = N_{CaO}$, $N_2 = N_{MgO}$, $N_3 = N_{MnO}$, $N_4 = N_{FeO}$,

$N_5 = N_{Fe_2O_3}$, $N_6 = N_{P_2O_5}$, $N_7 = N_{SiO_2}$, $N_8 = N_{CaFe_2O_4}$,

$N_9 = N_{Ca_2Fe_2O_5}$, $N_{10} = N_{MgFe_2O_4}$, $N_{11} = N_{MnFe_2O_4}$,

$N_{12} = N_{Fe_3O_4}$, $N_{13} = N_{2CaO\cdot P_2O_5}$, $N_{14} = N_{3CaO\cdot P_2O_5}$,

$N_{15} = N_{4CaO\cdot P_2O_5}$, $N_{16} = N_{2MgO\cdot P_2O_5}$, $N_{17} = N_{3MgO\cdot P_2O_5}$,

$N_{18} = N_{3MnO\cdot P_2O_5}$, $N_{19} = N_{3FeO\cdot P_2O_5}$, $N_{20} = N_{4FeO\cdot P_2O_5}$,

$N_{21} = N_{CaSiO_3}$, $N_{22} = N_{Ca_2SiO_4}$, $N_{23} = N_{Ca_3SiO_5}$,

$N_{24} = N_{MgSiO_3}$, $N_{25} = N_{Mg_2SiO_4}$, $N_{26} = N_{MnSiO_3}$,

$N_{27} = N_{Mn_2SiO_4}$, $N_{28} = N_{Fe_2SiO_4}$, $N_{29} = N_{CaO\cdot MgO\cdot SiO_2}$,

$N_{30} = N_{CaO\cdot MgO\cdot 2SiO_2}$, $N_{31} = N_{2CaO\cdot MgO\cdot 2SiO_2}$,

$N_{32} = N_{3CaO\cdot MgO\cdot 2SiO_2}$,

$\sum n$ = the sum of the amount of ions and molecules in equilibrium (in mol). As in this slag system, there are 14 compounds, and the chemical reactions and thermodynamic parameters have already been given in the above-mentioned, so only the expressions of equilibrium amount (in mol) are listed as

$$z_1 = 2K_1\frac{x_1y_1}{\sum n},\ z_2 = 4K_2\frac{x_1^2y_1}{(\sum n)^2},\ z_3 = 2K_3\frac{x_2y_1}{\sum n},$$

$$z_5 = 2K_5\frac{x_4y_1}{\sum n},\ z_{14} = 2K_{14}\frac{x_1y_3}{\sum n},\ z_{15} = 4K_{15}\frac{x_1^2y_3}{(\sum n)^2},$$

$$z_{16} = 8K_{16}\frac{x_1^3y_1}{(\sum n)^3},\ z_{17} = 2K_{17}\frac{x_2y_3}{\sum n},\ z_{18} = 4K_{18}\frac{x_2^2y_3}{(\sum n)^2},$$

$$z_{21} = 4K_{21}\frac{x_4^2y_3}{(\sum n)^2},\ z_{22} = 4K_{22}\frac{x_1x_2y_3}{(\sum n)^2},$$

$$z_{23} = 4K_{23}\frac{x_1x_2y_3^2}{(\sum n)^3},\ z_{24} = 8K_{24}\frac{x_1^2x_2y_3^2}{(\sum n)^4},$$

$$z_{25} = 16K_{25}\frac{x_1^3x_2y_3^2}{(\sum n)^5} \tag{27}$$

While for the compounds which have not been illustrated above, their chemical equilibria, expressions of equilibrium amount (in mol) and thermodynamic parameters are given in detail as follows:

$(Mn^{2+}+O^{2-})_{(s)}+Fe_2O_{3(s)}=MnFe_2O_{4(s)}$,

$$K_4 = \frac{N_{11}}{N_3N_5},\ z_4 = 2K_4\frac{x_3y_1}{\sum n} \tag{28}$$

$\Delta G^\circ = -35726 + 13.138\ T$ (J/mol) [12];

$2(Ca^{2+} + O^{2-}) + (P_2O_5) = (2CaO\cdot P_2O_5)$,

$$K_6 = \frac{N_{13}}{N_1^2N_2},\ z_6 = 4K_6\frac{x_1^2y^2}{(\sum n)^2} \tag{29}$$

$\Delta G^\circ = -120427.125 - 290.521T$ (J/mol) [6];

$3(Ca^{2+} + O^{2-}) + (P_2O_5) = (3CaO\cdot P_2O_5)$,

$$K_7 = \frac{N_{14}}{N_1^3N_2},\ z_7 = 8K_7\frac{x_1^3y_2}{(\sum n)^3} \tag{30}$$

$\Delta G^\circ = -694563.125 + 49.897\ T$ (J/mol) [6];

$4(Ca^{2+} + O^{2-}) + (P_2O_5) = (4CaO\cdot P_2O_5)$,

$$K_8 = \frac{N_{15}}{N_1^4N_2},\ z_8 = 16K_8\frac{x_1^4y_2}{(\sum n)^4} \tag{31}$$

$\Delta G^\circ = -822509.8 + 95.893\ T$ (J/mol) [6];

$2(Mg^{2+} + O^{2-}) + (P_2O_5) = (2MgO\cdot P_2O_5)$,

$$K_9 = \frac{N_{16}}{N_2^2N_2},\ z_9 = 4K_9\frac{x_2^2y_2}{(\sum n)^2} \tag{32}$$

$\Delta G^\circ = -168359.4 - 339.35T$ (J/mol) [6];

$3(Mg^{2+} + O^{2-}) + (P_2O_5) = (3MgO\cdot P_2O_5)$,

$$K_{10} = \frac{N_{17}}{N_2^3N_2},\ z_{10} = 8K_{10}\frac{x_2^3y_2}{(\sum n)^3} \tag{33}$$

$\Delta G^\circ = -486715.5 + 36.844\ T$ (J/mol) [6];

$3(Mn^{2+} + O^{2-}) + (P_2O_5) = (3MnO\cdot P_2O_5)$,

$$K_{11} = \frac{N_{18}}{N_3^3N_2},\ z_{11} = 8K_{11}\frac{x_3^3y_2}{(\sum n)^3} \tag{34}$$

$\Delta G^\circ = -526421.411 + 102.049\ T$ (J/mol) [6];

$3(Fe^{2+} + O^{2-}) + (P_2O_5) = (3FeO\cdot P_2O_5)$,

$$K_{12} = \frac{N_{19}}{N_4^3N_2},\ z_{12} = 8K_{12}\frac{x_4^3y_2}{(\sum n)^3} \tag{35}$$

$\Delta G^\circ = -430404 + 92.708\ T$ (J/mol) [6];

$4(Fe^{2+} + O^{2-}) + (P_2O_5) = (4FeO{\cdot}P_2O_5)$,

$$K_{13} = \frac{N_{20}}{N_4^2 N_2},\ z_{13} = 16K_{13}\frac{x_4^4 y_2}{(\sum n)^4} \quad (36)$$

$\Delta G^\circ = -381831.469 + 47.367\,T$ (J/mol) [6];

$(Mn^{2+} + O^{2-}) + (SiO_2) = (MnSiO_3)$,

$$K_{19} = \frac{N_{26}}{N_3 N_7},\ z_{19} = 2K_{19}\frac{x_3 y_3}{\sum n} \quad (37)$$

$\Delta G^\circ = -30013 - 5.02T$ (J/mol) [14];

$2(Mn^{2+} + O^{2-}) + (SiO_2) = (Mn_2SiO_4)$,

$$K_{20} = \frac{N_{27}}{N_3^2 N_7},\ z_{20} = 4K_{20}\frac{x_3^2 y_3}{(\sum n)^2} \quad (38)$$

$\Delta G^\circ = -86670 + 16.81\,T$ (J/mol) [14].

Mass balance:

$$b_1 = x_1 + z_1 + 2z_2 + 2z_6 + 3z_7 + 4z_8 + z_{14} + 2z_{15} + 3z_{16} + z_{22} + z_{23} + 2z_{24} + 3z_{25} \quad (39)$$

$$b_2 = x_2 + z_3 + 2z_9 + 3z_{10} + z_{17} + 2z_{18} + z_{22} + z_{23} + z_{24} + z_{25} \quad (40)$$

$$b_3 = x_3 + z_4 + 3z_{11} + z_{19} + 2z_{20} \quad (41)$$

$$b_4 = x_4 + z_5 + 3z_{12} + 4z_{13} + 2z_{21} \quad (42)$$

$$a_1 = y_1 + z_1 + z_2 + z_3 + z_4 + z_5 \quad (43)$$

$$a_2 = y_2 + z_6 + z_7 + z_8 + z_9 + z_{10} + z_{11} + z_{12} + z_{13} \quad (44)$$

$$a_3 = y_3 + z_{14} + z_{15} + z_{16} + z_{17} + z_{18} + z_{19} + z_{20} + z_{21} + z_{22} + 2z_{23} + 2z_{24} + 2z_{25} \quad (45)$$

$$\sum n = 2\sum_{i=1}^{4} x_i + \sum_{j=1}^{3} y_j + \sum_{k=1}^{25} z_k \quad (46)$$

Equations (27)-(46) as well as equations (21) and (22) are the calculating model of mass action concentration for the slag melt. Similarly, the desulphurization of MnO between the slag melt and liquid iron can be written as

$(Mn^{2+} + O^{2-}) + [S] = (Mn^{2+} + S^{2-}) + [O]$,

$$L_{MnS} = 8K_{MnS}N_{MnO}\frac{\sum n}{[O]} \quad (47)$$

Hence, the sulphur distribution coefficient between the slag melt and liquid iron is:

$$L_S = \frac{8(K_{CaS}N_{CaO} + K_{MgS}N_{MgO} + K_{MnS}N_{MnO} + K_{FeS}N_{FeO})\sum n}{[O]} \quad (48)$$

Using equilibrium sulphur distribution data between the slag melt and liquid iron from reference [15] as well as equations (27)-(46), the mass action concentration of the slag melt at different temperatures is calculated, then the equilibrium constants of desulphurization for the slag melt are regressed as

$K_{CaS} = 0.039996$, $K_{MnS} = 0.056268$,

$K_{FeS} = 0.044901$, $K_{MgS} = -0.03015$,

$R = 0.9825$, $F = 770$.

So, the sulphur distribution coefficient for the slag melt and liquid iron can be expressed by the following equation as

$$L_S = [8(0.039996N_{CaO} + 0.056268N_{MnO} + 0.044901N_{FeO} - 0.03015N_{MgO})\sum n]/[O\%].$$

The comparison of L_{SC} calculated with L_{SP} observed is shown in **figure 2**. It is seen from the figure that, though a small part of points shows some scatter, the overall agreement between the calculated and measured values is satisfactory. Therefore, the aforementioned calculating model can reflect the sulphur distribution characteristics between the slag melt and liquid iron. Also, K_{MgS} is negative.

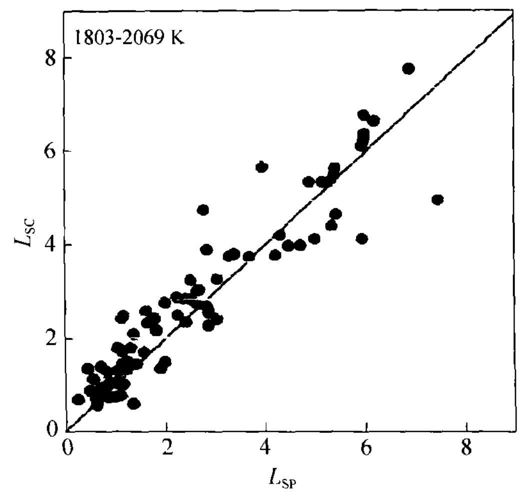

Figure 2 Comparison of the calculated L_{SC} values with the observed L_{SP} values at temperatures of 1803-2069 K.

3 Sulphur distribution between CaO-MgO-MnO-FeO-Fe$_2$O$_3$-Al$_2$O$_3$-P$_2$O$_5$-SiO$_2$ slag melt and liquid iron

In comparison with CaO-MgO-MnO-FeO-Fe_2O_3-P_2O_5-SiO_2 slag melt, and according to the phase diagrams [5] and the coexistence theory of slag structure [6], the additional structural units of this slag system are Al_2O_3, $3CaO{\cdot}Al_2O_3$, $12CaO{\cdot}7Al_2O_3$, $CaO{\cdot}Al_2O_3$, $CaO{\cdot}2Al_2O_3$, $CaO{\cdot}6Al_2O_3$, $MgO{\cdot}Al_2O_3$, $MnO{\cdot}Al_2O_3$, $FeO{\cdot}Al_2O_3$, $CaO{\cdot}Al_2O_3{\cdot}2SiO_2$, $2CaO{\cdot}Al_2O_3{\cdot}SiO_2$ and

$3Al_2O_3{\cdot}2SiO_2$.

Assuming the composition of the melt as

$b_1 = \sum n_{CaO}$, $b_2 = \sum n_{MgO}$, $b_3 = \sum n_{MnO}$, $b_4 = \sum n_{FeO}$,

$a_1 = \sum n_{Fe_2O_3}$, $a_2 = \sum n_{Al_2O_3}$, $a_3 = \sum n_{P_2O_5}$, $a_4 = \sum n_{SiO_2}$;

the amount equilibrium of every structural unit (in mol) expressed by the composition as

$x_1 = n_{CaO}$, $x_2 = n_{MgO}$, $x_3 = n_{MnO}$, $x_4 = n_{FeO}$, $y_1 = n_{Fe_2O_3}$,

$y_2 = n_{Al_2O_3}$, $y_3 = n_{P_2O_5}$, $y_4 = n_{SiO_2}$, $z_1 = n_{CaFe_2O_4}$,

$z_2 = n_{Ca_2Fe_2O_5}$, $z_3 = n_{MgFe_2O_4}$, $z_4 = n_{MnFe_2O_4}$, $z_5 = n_{Fe_3O_4}$,

$z_6 = n_{3CaO\cdot Al_2O_3}$, $z_7 = n_{12CaO\cdot 7Al_2O_3}$, $z_8 = n_{CaO\cdot Al_2O_3}$,

$z_9 = n_{CaO\cdot 2Al_2O_3}$, $z_{10} = n_{CaO\cdot 6Al_2O_3}$, $z_{11} = n_{MgO\cdot Al_2O_3}$,

$z_{12} = n_{MnO\cdot Al_2O_3}$, $z_{13} = n_{FeO\cdot Al_2O_3}$, $z_{14} = n_{2CaO\cdot P_2O_5}$,

$z_{15} = n_{3CaO\cdot P_2O_5}$, $z_{16} = n_{4CaO\cdot P_2O_5}$, $z_{17} = n_{2MgO\cdot P_2O_5}$,

$z_{18} = n_{3MgO\cdot P_2O_5}$ $z_{19} = n_{3MnO\cdot P_2O_5}$, $z_{20} = n_{3FeO\cdot P_2O_5}$,

$z_{21} = n_{4FeO\cdot P_2O_5}$, $z_{22} = n_{CaSiO_3}$, $z_{23} = n_{Ca_2SiO_4}$,

$z_{24} = n_{Ca_3SiO_5}$, $z_{25} = n_{MgSiO_3}$, $z_{26} = n_{Mg_2SiO_4}$, $z_{27} = n_{MnSiO_3}$,

$z_{28} = n_{Mn_2SiO_4}$, $z_{29} = n_{Fe_2SiO_4}$, $z_{30} = n_{CaMgSiO_4}$,

$z_{31} = n_{CaO\cdot MgO\cdot 2SiO_2}$, $z_{32} = n_{2CaO\cdot MgO\cdot 2SiO_2}$,

$z_{33} = n_{3CaO\cdot MgO\cdot 2SiO_2}$, $z_{34} = n_{CaO\cdot Al_2O_3\cdot 2SiO_2}$,

$z_{35} = n_{2CaO\cdot Al_2O_3\cdot SiO_2}$, $z_{36} = n_{3Al_2O_3\cdot 2SiO_2}$;

the mass action concentration of every structural unit after normalization as

$N_1 = N_{CaO}$, $N_2 = N_{MgO}$, $N_3 = N_{MnO}$, $N_4 = N_{FeO}$,

$N_5 = N_{Fe_2O_3}$, $N_6 = N_{Al_2O_3}$, $N_7 = N_{P_2O_5}$, $N_8 = N_{SiO_2}$,

$N_9 = N_{CaFe_2O_4}$, $N_{10} = N_{Ca_2Fe_2O_5}$, $N_{11} = N_{MgFe_2O_4}$,

$N_{12} = N_{MnFe_2O_4}$, $N_{13} = N_{Fe_3O_4}$, $N_{14} = N_{3CaO\cdot Al_2O_3}$,

$N_{15} = N_{12CaO\cdot 7Al_2O_3}$, $N_{16} = N_{CaO\cdot Al_2O_3}$, $N_{17} = N_{CaO\cdot 2Al_2O_3}$,

$N_{18} = N_{CaO\cdot 6Al_2O_3}$, $N_{19} = N_{MgO\cdot Al_2O_3}$, $N_{20} = N_{MnO\cdot Al_2O_3}$,

$N_{21} = N_{FeO\cdot Al_2O_3}$, $N_{22} = N_{2CaO\cdot P_2O_5}$, $N_{23} = N_{3CaO\cdot P_2O_5}$,

$N_{24} = N_{4CaO\cdot P_2O_5}$, $N_{25} = N_{2MgO\cdot P_2O_5}$, $N_{26} = N_{3MgO\cdot P_2O_5}$,

$N_{27} = N_{3MnO\cdot P_2O_5}$, $N_{28} = N_{3FeO\cdot P_2O_5}$, $N_{29} = N_{4FeO\cdot P_2O_5}$,

$N_{30} = N_{CaSiO_3}$, $N_{31} = N_{Ca_2SiO_4}$, $N_{32} = N_{Ca_3SiO_5}$,

$N_{33} = N_{MgSiO_3}$, $N_{34} = N_{Mg_2SiO_4}$, $N_{35} = N_{MnSiO_3}$,

$N_{36} = N_{Mn_2SiO_4}$, $N_{37} = N_{Fe_2SiO_4}$, $N_{38} = N_{CaO\cdot MgO\cdot SiO_2}$,

$N_{39} = N_{CaO\cdot MgO\cdot 2SiO_2}$, $N_{40} = N_{2CaO\cdot MgO\cdot 2SiO_2}$,

$N_{41} = N_{3CaO\cdot MgO\cdot 2SiO_2}$, $N_{42} = N_{CaO\cdot Al_2O_3\cdot 2SiO_2}$,

$N_{43} = N_{2CaO\cdot Al_2O_3\cdot SiO_2}$, $N_{44} = N_{3Al_2O_3\cdot 2SiO_2}$,

$\sum n$= the sum of the amount of ions and molecules in equilibrium (in mol).

As in this slag system, there are 25 compounds, and the chemical reactions and thermodynamic parameters have already been given in the above-mentioned, so similarly, only the expressions of equilibrium amount (in mol) are listed as

$$z_1 = 2K_1\frac{x_1y_1}{\sum n},\ z_2 = 4K_2\frac{x_1^2y_1}{(\sum n)^2},\ z_3 = 2K_3\frac{x_2y_1}{\sum n},$$

$$z_4 = 2K_4\frac{x_3y_1}{\sum n},\ z_5 = 2K_5\frac{x_4y_1}{\sum n},\ z_{14} = 4K_{14}\frac{x_1^2y_3}{(\sum n)^2},$$

$$z_{15} = 8K_{15}\frac{x_1^3y_3}{(\sum n)^3},\ z_{16} = 16K_{16}\frac{x_1^4y_3}{(\sum n)^4},$$

$$z_{17} = 4K_{17}\frac{x_2^2y_3}{(\sum n)^2},\ z_{18} = 8K_{18}\frac{x_2^3y_3}{(\sum n)^3},$$

$$z_{19} = 8K_{19}\frac{x_3^3y_3}{(\sum n)^3},\ z_{20} = 8K_{20}\frac{x_4^3y_3}{(\sum n)^3},$$

$$z_{21} = 16K_{21}\frac{x_4^4y_3}{(\sum n)^4},\ z_{22} = 2K_{22}\frac{x_1y_4}{\sum n},$$

$$z_{23} = 4K_{23}\frac{x_1^2y_4}{(\sum n)^2},\ z_{24} = 8K_{24}\frac{x_1^3y_4}{(\sum n)^3},$$

$$z_{25} = 2K_{25}\frac{x_2y_4}{\sum n},\ z_{26} = 4K_{26}\frac{x_2^2y_4}{(\sum n)^2},$$

$$z_{27} = 2K_{27}\frac{x_3y_4}{\sum n},\ z_{28} = 4K_{28}\frac{x_3^2y_4}{(\sum n)^2},$$

$$z_{29} = 4K_{29}\frac{x_4^2y_4}{(\sum n)^2},\ z_{30} = 4K_{30}\frac{x_1x_2y_4}{(\sum n)^2},$$

$$z_{31} = 4K_{31}\frac{x_1x_2y_4^2}{(\sum n)^3},\ z_{32} = 8K_{32}\frac{x_1^2x_2y_4^2}{(\sum n)^4},$$

$$z_{33} = 16K_{33}\frac{x_1^3x_2y_4^2}{(\sum n)^5} \qquad (49)$$

Accordingly, for the compounds which have not been illustrated above, their chemical equilibria, expressions of equilibrium amount and thermodynamic parameters are given as follows:

$3(Ca^{2+} + O^{2-})_{(S)} + Al_2O_{3(S)} = 3CaO{\cdot}Al_2O_{3(S)}$,

$$K_6 = \frac{N_{14}}{N_1^3N_6},\ z_6 = 8K_6\frac{x_1^3y_2}{(\sum n)^3} \qquad (50)$$

$\Delta G^{\circ} = -17000 - 32.0\ T$ (J/mol) [16];

$12(Ca^{2+} + O^{2-})_{(S)} + 7Al_2O_{3(S)} = 12CaO{\cdot}7Al_2O_{3(S)}$,

$$K_7 = \frac{N_{15}}{N_1^{12}N_6^7},\ z_7 = 4096K_7\frac{x_1^{12}y_2^7}{(\sum n)^{18}} \qquad (51)$$

$\Delta G^\circ = -86100 - 205.1T$, J/mol [16];

$(Ca^{2+} + O^{2-})_{(S)} + Al_2O_{3(S)} = CaO \cdot Al_2O_{3(S)}$,

$$K_8 = \frac{N_{16}}{N_1 N_6},\ z_8 = 2K_8 \frac{x_1 y_2}{\sum n} \tag{52}$$

$\Delta G^\circ = -18120 - 18.62\,T$ (J/mol) [16];

$(Ca^{2+} + O^{2-})_{(S)} + 2Al_2O_{3(S)} = CaO \cdot 2Al_2O_{3(S)}$,

$$K_9 = \frac{N_{17}}{N_1 N_6^2},\ z_9 = 2K_9 \frac{x_1 y_2^2}{(\sum n)^2} \tag{53}$$

$\Delta G^\circ = -16400 - 26.8\,T$ (J/mol) [16];

$(Ca^{2+} + O^{2-})_{(S)} + 6Al_2O_{3(S)} = CaO \cdot 6Al_2O_{3(S)}$,

$$K_{10} = \frac{N_{18}}{N_1 N_6^6},\ z_{10} = 2K_{10} \frac{x_1 y_2^6}{(\sum n)^6} \tag{54}$$

$\Delta G^\circ = -17430 - 37.2\,T$ (J/mol) [16];

$(Mg^{2+} + O^{2-})_{(S)} + Al_2O_{3(S)} = MgO \cdot Al_2O_{3(S)}$,

$$K_{11} = \frac{N_{19}}{N_2 N_6},\ z_{11} = 2K_{11} \frac{x_2 y_2}{\sum n} \tag{55}$$

$\Delta G^\circ = -35530 - 2.09\,T$ (J/mol)[7];

$(Mn^{2+} + O^{2-})_{(S)} + Al_2O_{3(S)} = MnO \cdot Al_2O_{3(S)}$,

$$K_{12} = \frac{N_{20}}{N_3 N_6},\ z_{12} = 2K_{12} \frac{x_3 y_2}{\sum n} \tag{56}$$

$\Delta G^\circ = -45116 + 11.81\,T$ (J/mol) [17];

$(Fe^{2+} + O^{2-}) + Al_2O_{3(S)} = FeO \cdot Al_2O_{3(S)}$,

$$K_{13} = \frac{N_{21}}{N_4 N_6},\ z_{13} = 2K_{13} \frac{x_4 y_2}{\sum n} \tag{57}$$

$\Delta G^\circ = -33272.8 + 6.1028\,T$ (J/mol) [18];

$(Ca^{2+} + O^{2-}) + Al_2O_3 + 2(SiO_2) = (CaO \cdot Al_2O_3 \cdot 2SiO_2)$,

$$K_{34} = \frac{N_{42}}{N_1 N_6 N_8^2},\quad z_{34} = 2K_{34} \frac{x_1 y_2 y_4^2}{(\sum n)^3} \tag{58}$$

$\Delta G^\circ = -13816.44 - 55.266\,T$ (J/mol) [11];

$2(Ca^{2+} + O^{2-}) + Al_2O_3 + (SiO_2) = (2CaO \cdot Al_2O_3 \cdot SiO_2)$,

$$K_{35} = \frac{N_{43}}{N_1^2 N_6 N_8},\ z_{35} = 4K_{35} \frac{x_1^2 y_2 y_4}{(\sum n)^3} \tag{59}$$

$\Delta G^\circ = -61964.64 - 60.29\,T$ (J/mol) [11];

$3(Al_2O_3) + 2(SiO_2) = (3Al_2O_3 \cdot 2SiO_2)$,

$$K_{36} = \frac{N_{44}}{N_6^3 N_8^2},\ z_{36} = K_{36} \frac{y_2^3 y_4^2}{(\sum n)^4} \tag{60}$$

$\Delta G^\circ = -4354.27 - 10.467T$ (J/mol) [11].

Mass balance:

$$b_1 = x_1 + z_1 + 2z_2 + 3z_6 + 12z_7 + z_8 + z_9 + z_{10} + 2z_{14} + 3z_{15} + 4z_{16} + z_{22} + 2z_{23} + 3z_{24} + z_{30} + z_{31} + 2z_{32} + 3z_{33} + z_{34} + 2z_{35} \tag{61}$$

$$b_2 = x_2 + z_3 + z_{11} + 2z_{17} + 3z_{18} + z_{25} + 2z_{26} + z_{30} + z_{31} + z_{32} + z_{33} \tag{62}$$

$$b_3 = x_3 + z_4 + z_{12} + 3z_{19} + z_{27} + 2z_{28} \tag{63}$$

$$b_4 = x_4 + z_5 + z_{13} + 3z_{20} + 4z_{21} + 2z_{29} \tag{64}$$

$$a_1 = y_1 + z_1 + z_2 + z_3 + z_4 + z_5 \tag{65}$$

$$a_2 = y_2 + z_6 + 7z_7 + z_8 + 2z_9 + 6z_{10} + z_{11} + z_{12} + z_{13} + z_{34} + z_{35} + 3z_{36} \tag{66}$$

$$a_3 = y_3 + z_{14} + z_{15} + z_{16} + z_{17} + z_{18} + z_{19} + z_{20} + z_{21} \tag{67}$$

$$a_4 = y_4 + z_{22} + z_{23} + z_{24} + z_{25} + z_{26} + z_{27} + z_{28} + z_{29} + z_{30} + 2z_{31} + 2z_{32} + 2z_{33} + 2z_{34} + z_{35} + 2z_{36} \tag{68}$$

$$\sum n = 2\sum_{i=1}^{4} x_i + \sum_{j=1}^{4} y_j + \sum_{k=1}^{36} z_k \tag{69}$$

Equations (49)-(69) as well as equations (21) and (22) are the calculating model of mass action concentration for this slag system. The sulphur distribution coefficient between the slag melt and liquid iron can be also expressed by equation (48). Using equilibrium sulphur distribution data between the slag melt and liquid iron from reference [19] as well as the corresponding calculating model of mass action concentration, the mass action concentration of the slag melt at different temperatures is calculated, then the equilibrium constants of desulphurization for the slag melt are regressed as

$K_{CaS} = 0.018622$, $K_{MnS} = 0.015441$, $K_{FeS} = 0.017475$,

$K_{MgS} = -0.00491$, $R = 0.9093$, $F = 25.465$.

So, the sulphur distribution coefficient for the slag melt and liquid iron can be expressed by the following equation:

$$L_S = [8(0.018622N_{CaO} + 0.015441N_{MnO} + 0.017475N_{FeO} - 0.00491N_{MgO})\sum n]/[O\%].$$

By using this equation, calculated values of the sulphur distribution coefficient between the slag melt and liquid iron L_{SC} are compared with the observed L_{SP} values as shown in **figure 3**. It is seen from the figure that agreement between them is good, attesting that the above-mentioned calculating model can reflect the sulphur distribution characteristics between the slag melt and liquid iron. At the same time, the value of K_{MgS} is also negative.

From the above-mentioned three examples, it can be concluded that the mass action law as well as the coexistence theory of slag structure is practical to formulate sulphur distribution models between multi-component (over 5 components) slag melts and liquid iron which can reflect the structural reality of the melts. The negative value of K_{MgS} is probably arisen from the insolubility of a portion of MgO in the slag melts and the formation of solid solution with CaO, MnO, FeO *etc.* As a result, MgO not only doesn't desulphurize metals, but also interferes with the desulphurization of CaO, MnO, FeO *etc.* Therefore, K_{MgS} is not an equilibrium constant, but is a value which represents the detrimental effect of MgO in the slag melts.

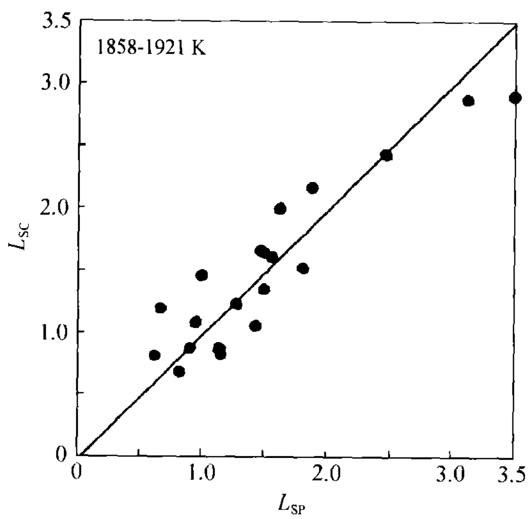

Figure 3 Comparison of the calculated L_{SC} values with the observed L_{SP} values at temperatures of 1858-1921 K.

In regard to the desulphurizing capability of basic oxides, in general, it can be arranged to the decreasing order as CaO→MnO→FeO→MgO. However, there are exceptions in the three examples cited, which is possibly due to the detrimental effect of MgO in one hand, and the analyzed oxygen content [O%] is the sum of soluble oxygen and that in nonmetallic inclusions, *i.e.*, T.[O], but not soluble oxygen only. In the other hand, because the desulphurization constants are only related to soluble oxygen, the positive values of K_{MgS} given in references [3,4] are probably the results of equilibrium experiments between simple oxide systems and gases, and they are different with equilibrium experiments between multicomponent slag melts and liquid iron. For this reason, the above-mentioned K_{CaS}, K_{MnS} and K_{FeS} are not real equilibrium constants, but apparent in nature.

Finally, from the three examples, no evident difference is found between apparent desulphurization constants at different temperatures, this is probably due to the negligible effect of temperature on desulphurization reactions of liquid iron with slag melts. However, this problem should be investigated further.

4 Conclusions

(1) The calculating models of mass action concentration for CaO-MgO-FeO-Fe_2O_3-SiO_2, CaO-MgO-MnO-FeO-Fe_2O_3-P_2O_5-SiO_2 and CaO-MgO-MnO-FeO-Fe_2O_3-Al_2O_3-P_2O_5-SiO_2 slag systems are formulated, and the sulphur distribution coefficient between the slag melts and liquid iron L_S is deduced. Between the first slag melt and liquid iron L_S can be expressed as

$$L_S = \frac{8(K_{CaS}N_{CaO} + K_{FeS}N_{FeO} - K_{MgS}N_{MgO})\sum n}{[O\%]},$$

while that between the second as well as third slag melts and liquid iron as

$$L_S = \frac{8(K_{CaS}N_{CaO} + K_{MnS}N_{MnO} + K_{FeS}N_{FeO} - K_{MgS}N_{MgO})\sum n}{[O\%]}$$

(2) Basic oxides CaO, MnO and FeO promote desulphurization, while MgO is detrimental to it.

(3) The mass action law as well as the coexistence theory of slag structure is practical to formulate the sulphur distribution model between multicomponent (over 5 components) slag melts and liquid iron which can reflect the structural reality of the melts.

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