$CaO-MgO-FeO-Fe_2O_3-SiO_2$炼钢渣系磷分配比的热力学模型

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摘 要 基于炉渣离子-分子共存理论(IMCT)建立了$CaO-MgO-FeO-Fe_2O_3-SiO_2$渣系的磷分配比预报模型，即IMCT-$L_P$模型. 比较了该渣系在1823～1873 K时实测的磷分配比、IMCT-L_P模型预报的磷分配比及其他6种磷分配比模型的计算结果. 与实测值和其他磷分配比模型预报结果相比，由IMCT-L_P模型预报的$CaO-MgO-FeO-Fe_2O_3-SiO_2$渣系的磷分配比更精确. 本文建立的IMCT-$L_P$模型不仅可计算该渣系的磷分配比，而且可计算该渣系中碱性离子对($Ca^{2+}+O^{2-}$)、($Mg^{2+}+O^{2-}$)和($Fe^{2+}+O^{2-}$)各自的磷分配比.

关键词 炼钢；渣系；脱磷；碱性氧化物；热力学模型
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Thermodynamic model of the phosphorus distribution ratio of $CaO-MgO-FeO-Fe_2O_3-SiO_2$ steelmaking slags

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ABSTRACT A thermodynamic model of the phosphorus distribution ratio (L_P) of $CaO-MgO-FeO-Fe_2O_3-SiO_2$ steelmaking slags was developed based on the ion and molecule coexistence theory (IMCT) of slags and verified by experimental data. The predicted phosphorus distribution ratio of $CaO-MgO-FeO-Fe_2O_3-SiO_2$ steelmaking slags in a temperature range of 1823 to 1873 K by the developed IMCT-L_P model is more accurate than the measured as well as the predicted phosphorus distribution by other phosphorus distribution models. The developed IMCT-L_P model can calculate not only the total phosphorus distribution of the slags but also the respective phosphorus distribution of ion pairs ($Ca^{2+}+O^{2-}$), ($Mg^{2+}+O^{2-}$), and ($Fe^{2+}+O^{2-}$) in the slags.

KEY WORDS steelmaking; slags; phosphorus removal; basic oxides; thermodynamic models

磷分配比(L_P)是表征炉渣脱磷能力的重要参数. 自20世纪30年代开始[1-3]，为了对炉渣氧化脱磷能力有精确的表征，人们对炉渣氧化脱磷进行了大量研究[1-18]并建立诸多渣系的L_P预报模型，比如Healy模型[10]、Suito模型[11-12]、Sommerville模型[5,13]和Balajiva模型[2]. 然而，上述模型都是在实测的磷分配比基础上通过数学回归拟合得到，不能很好地表现出脱磷的机理；同时由某一组实验数据回归拟合出的公式应用于其他渣系时，往往出现较大的误差，甚至当该公式应用于不同作者的同一渣

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系实验数据时,也出现较大的误差.

基于炉渣离子–分子共存理论(ion and molecule coexistence theory, IMCT)[19–24],本文建立了 $CaO-MgO-FeO-Fe_2O_3-SiO_2$ 渣系的磷分配比 L_P 预报模型,即 IMCT–L_P 模型. 通过实测的该渣系磷分配比 L_P[8,25] 与 IMCT–L_P 模型计算的 L_P 比较,以及与 Healy 模型[10]、Suito 模型[11–12]、Sommerville 模型[3,13]及 Balajiva 模型[2]六种磷分配比 L_P 预报模型结果相比较,验证了本文建立的 IMCT–L_P 模型的合理性. 本文的最终目的是开发一种基于炉渣离子–分子共存理论[19–24]的适合于多种渣系的 IMCT–L_P 预报模型,进而提供一种具有良好脱磷能力的炉渣成分设计新方法.

1　磷分配比模型

根据炉渣离子–分子共存理论,$CaO-MgO-FeO-Fe_2O_3-SiO_2$ 渣系与钢液间的脱磷反应可由氧化渣系中所有碱性离子对($Ca^{2+}+O^{2-}$)、($Mg^{2+}+O^{2-}$)和($Fe^{2+}+O^{2-}$)表征,这些碱性离子对与炉渣中铁氧化物 Fe_tO 反应生成八种脱磷产物 P_2O_5、$3FeO·P_2O_5$、$4FeO·P_2O_5$、$2CaO·P_2O_5$、$3CaO·P_2O_5$、$4CaO·P_2O_5$、$2MgO·P_2O_5$ 和 $3MgO·P_2O_5$. 其反应式如下所示:

$$2[P]+5(Fe_tO)=(P_2O_5)+5t[Fe],$$
$$\Delta_r G^{\ominus}_{m,P_2O_5}=-122412+312.522T,J·mol^{-1};\quad(1)$$

$$2[P]+5(Fe_tO)+3(Fe^{2+}+O^{2-})=(3FeO·P_2O_5)+5t[Fe],$$
$$\Delta_r G^{\ominus}_{m,3FeO·P_2O_5}=-552816+405.230T,J·mol^{-1};\quad(2)$$

$$2[P]+5(Fe_tO)+4(Fe^{2+}+O^{2-})=(4FeO·P_2O_5)+5t[Fe],$$
$$\Delta_r G^{\ominus}_{m,4FeO·P_2O_5}=-504243+359.889T,J·mol^{-1};\quad(3)$$

$$2[P]+5(Fe_tO)+2(Ca^{2+}+O^{2-})=(2CaO·P_2O_5)+5t[Fe],$$
$$\Delta_r G^{\ominus}_{m,2CaO·P_2O_5}=-707619+347.960T,J·mol^{-1};\quad(4)$$

$$2[P]+5(Fe_tO)+3(Ca^{2+}+O^{2-})=(3CaO·P_2O_5)+5t[Fe],$$
$$\Delta_r G^{\ominus}_{m,3CaO·P_2O_5}=-832302+318.672T,J·mol^{-1};\quad(5)$$

$$2[P]+5(Fe_tO)+4(Ca^{2+}+O^{2-})=(4CaO·P_2O_5)+5t[Fe],$$
$$\Delta_r G^{\ominus}_{m,4CaO·P_2O_5}=-783768+309.049T,J·mol^{-1};\quad(6)$$

$$2[P]+5(Fe_tO)+2(Mg^{2+}+O^{2-})=(2MgO·P_2O_5)+5t[Fe],$$
$$\Delta_r G^{\ominus}_{m,2MgO·P_2O_5}=45957-26.835T,J·mol^{-1};\quad(7)$$

$$2[P]+5(Fe_tO)+3(Mg^{2+}+O^{2-})=(3MgO·P_2O_5)+5t[Fe],$$
$$\Delta_r G^{\ominus}_{m,3MgO·P_2O_5}=-511389+272.230T,J·mol^{-1}\quad(8)$$

根据炉渣离子–分子共存理论[19–24],式(1)~(8)相应的反应平衡常数可表示为:

$$K^{\ominus}_{P_2O_5}=\frac{a_{P_2O_5}a_{Fe}^{5t}}{a_{Fe_tO}^{5}a_{P}^{2}}=\frac{N_{P_2O_5}\times 1}{N_{Fe_tO}^{5}[\%P]^2f_P^2}=\frac{[(\%P_2O_5)_{P_2O_5}/M_{P_2O_5}]/\sum n_i}{N_{Fe_tO}^{5}[\%P]^2f_P^2},\quad(9)$$

$$K^{\ominus}_{3FeO·P_2O_5}=\frac{a_{3FeO·P_2O_5}a_{Fe}^{5t}}{a_{Fe_tO}^{5}a_{FeO}^{3}a_{P}^{2}}=\frac{N_{3FeO·P_2O_5}\times 1}{N_{Fe_tO}^{5}N_{FeO}^{3}[\%P]^2f_P^2}=\frac{[(\%P_2O_5)_{3FeO·P_2O_5}/M_{P_2O_5}]/\sum n_i}{N_{Fe_tO}^{5}N_{FeO}^{3}[\%P]^2f_P^2},\quad(10)$$

$$K^{\ominus}_{4FeO·P_2O_5}=\frac{a_{4FeO·P_2O_5}a_{Fe}^{t}}{a_{Fe_tO}^{5}a_{FeO}^{4}a_{P}^{2}}=\frac{N_{4FeO·P_2O_5}\times 1}{N_{Fe_tO}^{5}N_{FeO}^{4}[\%P]^2f_P^2}=\frac{[(\%P_2O_5)_{4FeO·P_2O_5}/M_{P_2O_5}]/\sum n_i}{N_{Fe_tO}^{5}N_{FeO}^{4}[\%P]^2f_P^2},\quad(11)$$

$$K^{\ominus}_{2CaO·P_2O_5}=\frac{a_{2CaO·P_2O_5}a_{Fe}^{5t}}{a_{Fe_tO}^{5}a_{CaO}^{2}a_{P}^{2}}=\frac{N_{2CaO·P_2O_5}\times 1}{N_{Fe_tO}^{5}N_{CaO}^{2}[\%P]^2f_P^2}=\frac{[(\%P_2O_5)_{2CaO·P_2O_5}/M_{P_2O_5}]/\sum n_i}{N_{Fe_tO}^{5}N_{CaO}^{2}[\%P]^2f_P^2},\quad(12)$$

$$K^{\ominus}_{3CaO·P_2O_5}=\frac{a_{3CaO·P_2O_5}a_{Fe}^{5t}}{a_{Fe_tO}^{5}a_{CaO}^{3}a_{P}^{2}}=\frac{N_{3CaO·P_2O_5}\times 1}{N_{Fe_tO}^{5}N_{CaO}^{3}[\%P]^2f_P^2}=\frac{[(\%P_2O_5)_{3CaO·P_2O_5}/M_{P_2O_5}]/\sum n_i}{N_{Fe_tO}^{5}N_{CaO}^{3}[\%P]^2f_P^2},\quad(13)$$

$$K^{\ominus}_{4CaO·P_2O_5}=\frac{a_{4CaO·P_2O_5}a_{Fe}^{5t}}{a_{Fe_tO}^{5}a_{CaO}^{4}a_{P}^{2}}=\frac{N_{4CaO·P_2O_5}\times 1}{N_{Fe_tO}^{5}N_{CaO}^{4}[\%P]^2f_P^2}=$$

$$\frac{[(\%P_2O_5)_{4CaO\cdot P_2O_5}/M_{P_2O_5}]/\sum n_i}{N_{Fe_tO}^5 N_{CaO}^4 [\%P]^2 f_P^2}, \tag{14}$$

$$K_{2MgO\cdot P_2O_5}^{\ominus}=\frac{a_{2MgO\cdot P_2O_5}a_{Fe}^{5t}}{a_{Fe_tO}^5 a_{MgO}^2 a_P^2}=\frac{N_{2MgO\cdot P_2O_5}\times 1}{N_{Fe_tO}^5 N_{MgO}^2 [\%P]^2 f_P^2}=$$

$$\frac{[(\%P_2O_5)_{2MgO\cdot P_2O_5}/M_{P_2O_5}]/\sum n_i}{N_{Fe_tO}^5 N_{MgO}^2 [\%P]^2 f_P^2}, \tag{15}$$

$$K_{3MgO\cdot P_2O_5}^{\ominus}=\frac{a_{3MgO\cdot P_2O_5}a_{Fe}^{5t}}{a_{Fe_tO}^5 a_{MgO}^3 a_P^2}=\frac{N_{3MgO\cdot P_2O_5}\times 1}{N_{Fe_tO}^5 N_{MgO}^3 [\%P]^2 f_P^2}=$$

$$\frac{[(\%P_2O_5)_{3MgO\cdot P_2O_5}/M_{P_2O_5}]/\sum n_i}{N_{Fe_tO}^5 N_{MgO}^3 [\%P]^2 f_P^2}. \tag{16}$$

式中，$K_i^{\ominus}$ 为炉渣中碱性组元脱磷反应的平衡常数，a_i为组元活度，N_i为组元质量作用浓度，f_i 为组元活度系数，M_i为组元相对分子质量，$\sum n_i$ 为基于炉渣离子–分子共存理论[19-24] 所计算的 100 g 该渣系中所有结构单元总平衡物质的量，mol. 根据式(9)~(16)，在炉渣中有铁氧化物存在的情况下，碱性组元各自的磷分配比 $L_{P,i}$可表示如下：

$$L_{P,P_2O_5}=\frac{(\%P_2O_5)_{P_2O_5}}{[\%P]^2}=M_{P_2O_5}K_{P_2O_5}^{\ominus}N_{Fe_tO}^5 f_P^2\sum n_i, \tag{17}$$

$$L_{P,3FeO\cdot P_2O_5}=\frac{(\%P_2O_5)_{3FeO\cdot P_2O_5}}{[\%P]^2}=$$

$$M_{P_2O_5}K_{3FeO\cdot P_2O_5}^{\ominus}N_{Fe_tO}^5 N_{FeO}^3 f_P^2\sum n_i, \tag{18}$$

$$L_{P,4FeO\cdot P_2O_5}=\frac{(\%P_2O_5)_{4FeO\cdot P_2O_5}}{[\%P]^2}=$$

$$M_{P_2O_5}K_{4FeO\cdot P_2O_5}^{\ominus}N_{Fe_tO}^5 N_{FeO}^4 f_P^2\sum n_i, \tag{19}$$

$$L_{P,2CaO\cdot P_2O_5}=\frac{(\%P_2O_5)_{2CaO\cdot P_2O_5}}{[\%P]^2}=$$

$$M_{P_2O_5}K_{2CaO\cdot P_2O_5}^{\ominus}N_{Fe_tO}^5 N_{CaO}^2 f_P^2\sum n_i, \tag{20}$$

$$L_{P,3CaO\cdot P_2O_5}=\frac{(\%P_2O_5)_{3CaO\cdot P_2O_5}}{[\%P]^2}=$$

$$M_{P_2O_5}K_{3CaO\cdot P_2O_5}^{\ominus}N_{Fe_tO}^5 N_{CaO}^3 f_P^2\sum n_i, \tag{21}$$

$$L_{P,4CaO\cdot P_2O_5}=\frac{(\%P_2O_5)_{4CaO\cdot P_2O_5}}{[\%P]^2}=$$

$$M_{P_2O_5}K_{4CaO\cdot P_2O_5}^{\ominus}N_{Fe_tO}^5 N_{CaO}^4 f_P^2\sum n_i, \tag{22}$$

$$L_{P,2MgO\cdot P_2O_5}=\frac{(\%P_2O_5)_{2MgO\cdot P_2O_5}}{[\%P]^2}=$$

$$M_{P_2O_5}K_{2MgO\cdot P_2O_5}^{\ominus}N_{Fe_tO}^5 N_{MgO}^2 f_P^2\sum n_i, \tag{23}$$

$$L_{P,3MgO\cdot P_2O_5}=\frac{(\%P_2O_5)_{3MgO\cdot P_2O_5}}{[\%P]^2}=$$

$$M_{P_2O_5}K_{3MgO\cdot P_2O_5}^{\ominus}N_{Fe_tO}^5 N_{MgO}^3 f_P^2\sum n_i. \tag{24}$$

因此，CaO−MgO−FeO−Fe_2O_3−SiO_2 渣系和钢液间总的磷分配比可由式(17)~(24)计算得到：

$$L_P=L_{P,P_2O_5}+L_{P,3FeO\cdot P_2O_5}+L_{P,4FeO\cdot P_2O_5}+L_{P,2CaO\cdot P_2O_5}+$$
$$L_{P,3CaO\cdot P_2O_5}+L_{P,4CaO\cdot P_2O_5}+L_{P,2MgO\cdot P_2O_5}+L_{P,3MgO\cdot P_2O_5}=$$
$$\frac{(\%P_2O_5)_{P_2O_5}}{[\%P]^2}+\frac{(\%P_2O_5)_{3FeO\cdot P_2O_5}}{[\%P]^2}+$$
$$\frac{(\%P_2O_5)_{4FeO\cdot P_2O_5}}{[\%P]^2}+\frac{(\%P_2O_5)_{2CaO\cdot P_2O_5}}{[\%P]^2}+$$
$$\frac{(\%P_2O_5)_{3CaO\cdot P_2O_5}}{[\%P]^2}+\frac{(\%P_2O_5)_{4CaO\cdot P_2O_5}}{[\%P]^2}+$$
$$\frac{(\%P_2O_5)_{2MgO\cdot P_2O_5}}{[\%P]^2}+\frac{(\%P_2O_5)_{3MgO\cdot P_2O_5}}{[\%P]^2}=$$
$$M_{P_2O_5}N_{Fe_tO}^5 f_P^2(K_{P_2O_5}^{\ominus}+K_{3FeO\cdot P_2O_5}^{\ominus}N_{FeO}^3+$$
$$K_{4FeO\cdot P_2O_5}^{\ominus}N_{FeO}^4+K_{2CaO\cdot P_2O_5}^{\ominus}N_{CaO}^2+K_{3CaO\cdot P_2O_5}^{\ominus}N_{CaO}^3+$$
$$K_{4CaO\cdot P_2O_5}^{\ominus}N_{CaO}^4+K_{2MgO\cdot P_2O_5}^{\ominus}N_{MgO}^2+K_{3MgO\cdot P_2O_5}^{\ominus}N_{MgO}^3)\sum n_i. \tag{25}$$

式(25)即为 CaO−MgO−FeO−Fe_2O_3−SiO_2 渣系的磷分配比 L_P 预报模型. 根据计算出的 N_i、$\sum n_i$、$K_i^{\ominus}$ 和 f_P，可计算出渣系总的磷分配比 L_P 和碱性组元各自的磷分配比 $L_{P,i}$. 式(1)~(8)中脱磷反应的标准摩尔 Gibbs 自由能 $\Delta_r G_{m,i}^{\ominus}$总结于表 1 中.

2 结果与讨论

2.1 IMCT−L_P 预报模型与实测值的比较

为了验证本文建立的如式(25)所示的CaO−MgO−FeO−Fe_2O_3−SiO_2 渣系中 IMCT−L_P 的准确性，对该渣系由实测的 L_P[8,25]($\lg L_{P,mess}$)与 IMCT−L_P 模型的计算结果($\lg L_{P,cal}$)进行了比较. 需要说明的是，式(25)所示的 IMCT−L_P 模型不涉及任何数学拟合参数，并且是与不同作者[8,25] 所测得的 L_P 进行比较，其结果如图 1 所示.

由图 1 可以看出，IMCT−L_P 计算值和实测值 L_P 有良好的线性对应关系，而图 1(a)中 IMCT−L_P 计算值和实测值 L_P 的线性对应关系却又明显好于图 1(b)中 IMCT−L_P 计算值和实测值 L_P 的线性对应关系. 其主要原因是 Basu 等[8] 的实测数据完成于 2006 年附近，其实验精确度高于 Ting 等[25] 在 20

表 1　八种脱磷反应的标准摩尔 Gibbs 自由能

Table 1　Standard molar Gibbs free energy of 8 dephosphorization reactions

化学反应方程式	$\Delta_r G^{\ominus}_{m,i}/(J\cdot mol^{-1})$	文献来源
$1/2P_2 = [P]$	$-157700+5.4T$	[26]
$1/2O_2 = [O]$	$-117110-3.39T$	[26]
$2[P]+5[O] = (P_2O_5)(l)$	$-702912+556.472T$	[27]
$P_2+5/2O_2 = (P_2O_5)(l)$	$-1603862+550.322T$	[26-27]
$t[Fe]+[O] = (Fe_tO)$	$-116100+48.79T$	[28]
$2[P]+5(Fe_tO) = (P_2O_5)+5t[Fe]$	$-122412+312.522T$	本文
$3(FeO)+(P_2O_5) = (3FeO\cdot P_2O_5)$	$-430404+92.708T$	[2]
$2[P]+5(Fe_tO)+3(Fe^{2+}+O^{2-}) = (3FeO\cdot P_2O_5)+5t[Fe]$	$-552816+405.23T$	本文
$4(Fe^{2+}+O^{2-})+(P_2O_5) = (4FeO\cdot P_2O_5)$	$-381831+47.367T$	[2]
$2[P]+5(Fe_tO)+4(Fe^{2+}+O^{2-}) = (4FeO\cdot P_2O_5)+5t[Fe]$	$-504243+359.889T$	本文
$2(CaO)+P_2+5/2O_2 = (2CaO\cdot P_2O_5)(s)$	$-2189069+585.76T$	[22]
$2(CaO)+(P_2O_5)(l) = (2CaO\cdot P_2O_5)(s)$	$-585207+35.438T$	[22]
$2[P]+5(Fe_tO)+2(Ca^{2+}+O^{2-}) = (2CaO\cdot P_2O_5)+5t[Fe]$	$-707619+347.96T$	本文
$3(CaO)+P_2+5/2O_2 = (3CaO\cdot P_2O_5)(s)$	$-2313752+556.472T$	[22]
$3(CaO)+(P_2O_5)(l) = (3CaO\cdot P_2O_5)(s)$	$-709890+6.15T$	[22]
$2[P]+5(Fe_tO)+3(Ca^{2+}+O^{2-}) = (3CaO\cdot P_2O_5)(s)+5t[Fe]$	$-832302+318.672T$	本文
$4(CaO)+(P_2O_5)(l) = (4CaO\cdot P_2O_5)(l)$	$-661356-3.473T$	[29]
$2[P]+5(Fe_tO)+4(Ca^{2+}+O^{2-}) = (4CaO\cdot P_2O_5)+5t[Fe]$	$-783768+309.049T$	本文
$2(Mg^{2+}+O^{2-})+(P_2O_5) = (2MgO\cdot P_2O_5)$	$168369-339.357T$	[2]
$2[P]+5(Fe_tO)+2(Mg^{2+}+O^{2-}) = (2MgO\cdot P_2O_5)+5t[Fe]$	$45957-26.835T$	本文
$3(MgO)+P_2+5/2O_2 = (3MgO\cdot P_2O_5)(s)$	$-1992839+510.0296T$	[22]
$3(MgO)+(P_2O_5) = (3MgO\cdot P_2O_5)(s)$	$-388977-40.283T$	[22]
$2[P]+5(Fe_tO)+3(Mg^{2+}+O^{2-}) = (3MgO\cdot P_2O_5)+5t[Fe]$	$-511389+272.230T$	本文

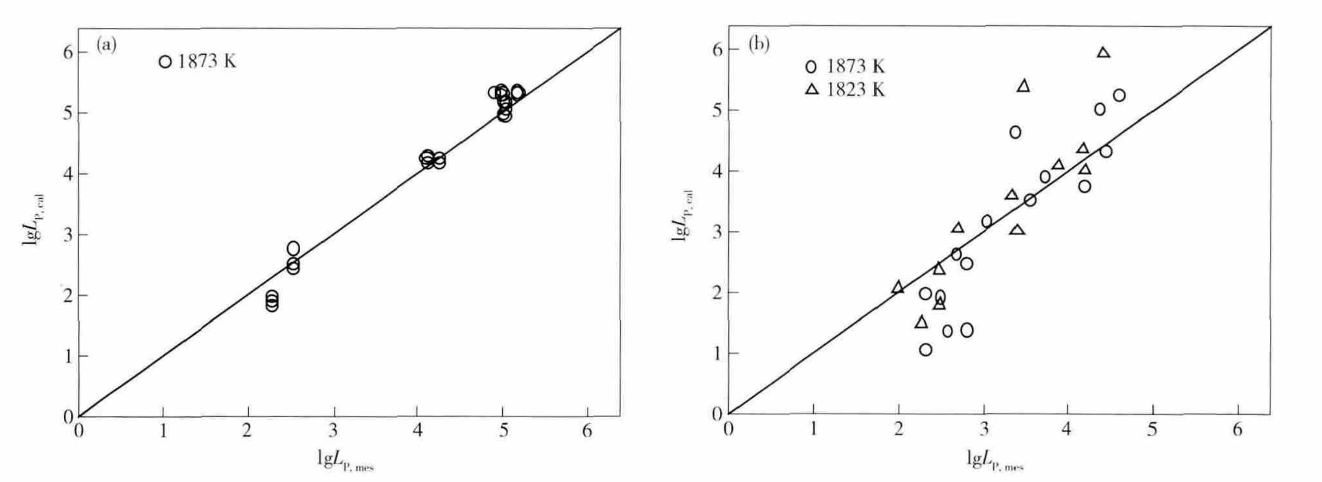

图 1　$CaO-MgO-FeO-Fe_2O_3-SiO_2$ 渣系中实测磷分配比与本文基于 IMCT 模型计算的磷分配比的关系. (a) Basu 等[8] 实测; (b) Ting 等[25] 实测

Fig. 1　Comparison between calculated and measured phosphorus distribution ratio of $CaO-MgO-FeO-Fe_2O_3-SiO_2$ slags: (a) Results of Basu et al.[8]; (b) Results of Ting et al.[25]

世纪 80 年代测定的数据. 这表明本文 IMCT—L_P 模型可以准确预报出 $CaO-MgO-FeO-Fe_2O_3-SiO_2$ 渣系中的磷分配比.

2.2 不同模型计算磷分配比

为了进一步比较 IMCT-L_P 模型的适用性，本文选择 Basu 等[8] 的 L_P 实测数值（$\lg L_{P,cal}$）作为参考对象，将 IMCT—L_P 模型与 Healy 模型[10]、Suito 模型[11-12]、Sommerville 模型[5,13] 和 Balajiva 模型[2] 磷分配比 L_P 预报模型结果（$\lg L_{P,cal}$）进行比较，如图 2 所示.

通过图 2 可以看出，IMCT—L_P 模型和 Healy 模型[10] 的 L_P 预报精确度高于其他模型，然而 Healy 模型涉及到较多人工拟合参数，不能很好反映出脱磷机理，Suito 模型[11-12]、Sommerville 模型[5,13] 和 Balajiva 模型[2] 中数学拟合公式却未达到精确预报磷分配比的目的，因此可以推论出人工拟合参数方法需不断优化其参数才能达到精确预报结果的目的，其适用性不如 IMCT—L_P 模型.

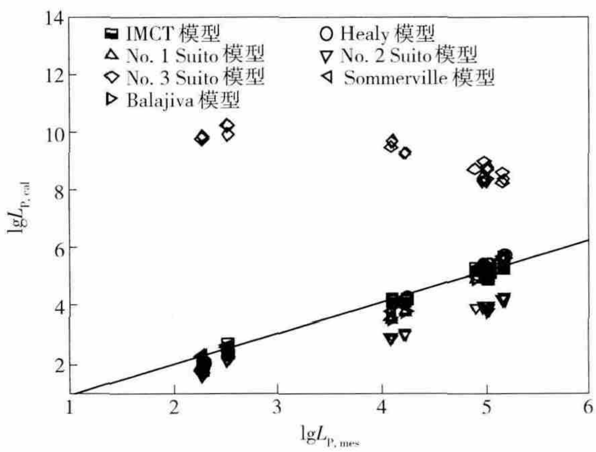

图 2 七种模型计算的 $CaO-MgO-FeO-Fe_2O_3-SiO_2$ 渣系中磷分配比与实测的该渣系磷分配比的比较

Fig. 2 Comparison between measured L_P and calculated L_P logarithms of $CaO-MgO-FeO-Fe_2O_3-SiO_2$ slags by seven prediction models

2.3 碱性组元的贡献

目前测量炉渣磷分配比的方法仅能测量出炉渣总的磷分配比，不能测量出具有脱磷能力碱性氧化物组元对渣系磷分配比的贡献率. IMCT—L_P 模型计算得到的 $CaO-MgO-FeO-Fe_2O_3-SiO_2$ 渣系中八种脱磷产物 P_2O_5、$3FeO\cdot P_2O_5$、$4FeO\cdot P_2O_5$、$2CaO\cdot P_2O_5$、$3CaO\cdot P_2O_5$、$4CaO\cdot P_2O_5$、$2MgO\cdot P_2O_5$ 和 $3MgO\cdot P_2O_5$ 的磷分配比 $L_{P,i}$ 与计算的该渣系总的磷分配比 L_P 的关系如图 3 所示.

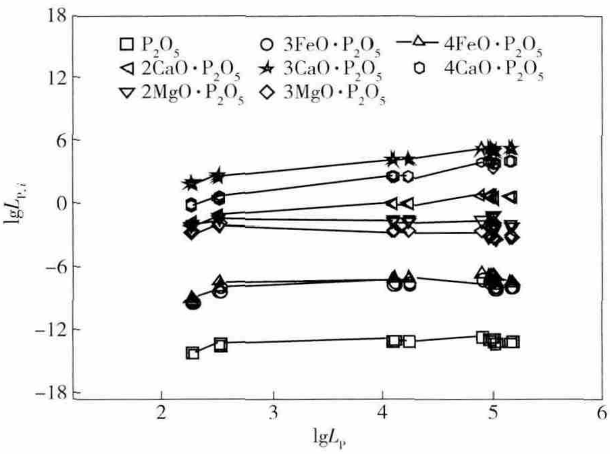

图 3 $CaO-MgO-FeO-Fe_2O_3-SiO_2$ 渣系中八种含 P_2O_5 的复杂分子对磷分配比的贡献

Fig. 3 Contribution of 8 structural units or complex molecules containing P_2O_5 on the L_P of $CaO-MgO-FeO-Fe_2O_3-SiO_2$ slags

显然，离子对（$Ca^{2+}+O^{2-}$）对 $CaO-MgO-FeO-Fe_2O_3-SiO_2$ 渣系的脱磷能力最大，MgO 的脱磷能力次之，FeO 的脱磷能力最低. 这一结果与 Suito 和 Inoue[30] 报道的脱磷能力贡献一致. 因此，离子对（$Ca^{2+}+O^{2-}$）或自由 CaO 对 $CaO-MgO-FeO-Fe_2O_3-SiO_2$ 渣系的脱磷贡献起决定性作用.

3 碱性组元质量分数的影响

$CaO-MgO-FeO-Fe_2O_3-SiO_2$ 渣系中碱性组元质量分数与 IMCT—L_P 模型预报的 L_P（$\lg L_{P,cal}$）和 Basu等[8] 实测的 L_P（$\lg L_{P,mes}$）的关系如图 4 所示. 可以看出，CaO 和 Fe_tO 含量增加以及 MgO 和 SiO_2 含量减少可有效增大 IMCT—L_P 模型预报的 L_P 和该渣系实测的 $L_{P,mes}$[8]. 同时，四种组元质量分数和 $L_{P,mes}$ 的拟合度与 IMCT—L_P 模型预报的 $L_{P,cal}^{IMCT}$ 的拟合度较好.

4 结论

（1）基于炉渣离子—分子共存理论建立的 IMCT—L_P 模型可准确预报 $CaO-MgO-FeO-Fe_2O_3-SiO_2$ 渣系的磷分配比，同时 IMCT—L_P 模型预报值比其他磷分配比模型预报结果更准确.

（2）建立的 IMCT—L_P 模型不仅可定量预报 $CaO-MgO-FeO-Fe_2O_3-SiO_2$ 渣系的总磷分配比，而且可预报该渣系中具有脱磷能力的碱性离子对（$Ca^{2+}+O^{2-}$）、（$Mg^{2+}+O^{2-}$）和（$Fe^{2+}+O^{2-}$）对该渣系总磷分配比的贡献.

（3）CaO 和 Fe_tO 含量增加以及 MgO 和 SiO_2 含量减少可有效增大 IMCT—L_P 模型预报的 $L_{P,cal}$ 和该

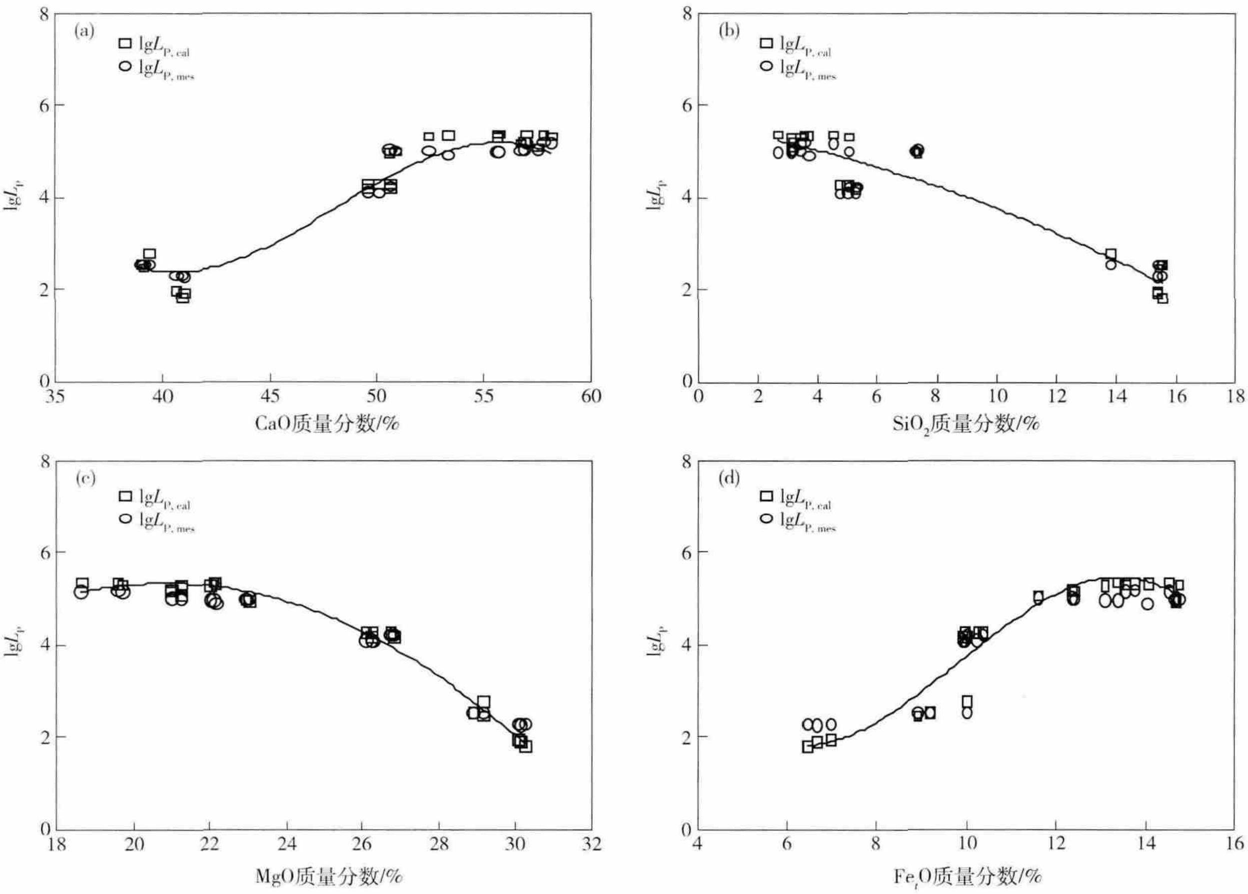

图 4　CaO—MgO—FeO—Fe_2O_3—SiO_2 渣系中不同组元的质量分数与 IMCT—L_P 模型计算的磷分配比 L_P 及 Basu 等[8] 测量的磷分配比 L_P 的关系. (a) CaO; (b) SiO_2; (c) MgO; (d) Fe_tO

Fig. 4　Change in phosphorus distribution of CaO—MgO—FeO—Fe_2O_3—SiO_2 slags calculated by the IMCT—L_P model and measured by Basu et al. [8] with the mass fraction of components: (a) CaO; (b) SiO_2; (c) MgO; (d) Fe_tO

渣系实测的 $L_{P,mes}$. 同时, 四种组元质量分数和 $L_{P,mes}$的拟合度与 IMCT—L_P 模型预报的 $L_{P,cal}$的拟合度较好.

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