**Supplementary Information**

Thermodynamic model for deoxidation of liquid steel considering strong metal–oxygen interaction in the quasichemical model framework

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# Appendix A. Deoxidation in liquid steel by Mg, La, and Zr

In continuation of the results discussed in **section [5.3](#sec_Ca)**, Figs. A.1–A.3 present the deoxidation equilibria of liquid steel by other strong deoxidizers, namely Mg, La, and Zr, respectively. The calculated [%O] in liquid steel deoxidized by Mg (Fig. A.1) [1–2] reasonably agrees with that of the present model. For the deoxidation by La (Fig A.2), the calculated $a\_{\overline{O}(wt\%)}$) shows good agreement with the data of Janke and Fischer [3]; however, the calculated [%O] is lower than the reported experimental data [4–5], similar to the case of Ce deoxidation. As for the deoxidation by Zr (Fig. A.3), the calculated [%O] is lower than the reported experimental findings [5–8], and the calculated $a\_{\overline{O}(wt\%)}$) agrees well with the data [6–7,9].



Fig. A.1. Deoxidation equilibria of Mg in liquid steel at 1600°C: [%O] as a function of [%Mg]. Experimental data were taken from [1–2].



Fig. A.2. Deoxidation equilibria of La in liquid steel at 1600°C: [%O] and $a\_{\overline{O}(wt\%)}$ (with respect to 1wt% standard state) as a function of [%La]. Experimental data were taken from [3–5]. Thermodynamic calculation reported in the literature is also shown [10].



Fig. A.3. Deoxidation equilibria of Zr in liquid steel at 1600°C: [%O] and $a\_{\overline{O}(wt\%)}$ (with respect to 1wt% standard state) as a function of [%Zr]. Experimental data were taken from [5–9]. Thermodynamic calculation reported in the literature is also shown [10].

# Appendix B. Deoxidation of liquid steel by Nb, V, and B

Deoxidation of liquids steel by Nb, V, and B was also described using the present model. The calculated results are shown in Figs. B.1–B.3.



Fig. B.1. Deoxidation equilibria of Nb in liquid steel at 1600°C: [%O] and $a\_{\overline{O}(wt\%)}$ (with respect to 1wt% standard state) as a function of [%Nb]. Experimental data were taken from [11–17]. Thermodynamic calculation reported in the literature is also shown.



Fig. B.2. Deoxidation equilibria of V in liquid steel at 1600°C: [%O] and $a\_{\overline{O}(wt\%)}$ (with respect to 1wt% standard state) as a function of [%V]. Experimental data were taken from [18–23]. Thermodynamic calculation reported in the literature is also shown [10].



Fig. B.3. Deoxidation equilibria of B in liquid steel at 1600°C: [%O] and $a\_{\overline{O}(wt\%)} $(with respect to 1wt% standard state) as a function of [%B]. Experimental data were taken from [20,24−25]. Thermodynamic calculation reported in the literature is also shown [10].

# Appendix C. Complex deoxidation in liquid Fe

In a $c$-component solution composed of M1-...-M*i*-...-M*c*-1-M*c*, where M1 is the solvent (Fe), M2 to M*c*-1 are deoxidizing elements (such as Al, Mn, Si, *etc.*), and M*c* is O, the Gibbs energy of the solution in Eq. (22) is extended as follows:

$G=\sum\_{i=1}^{c}n\_{i}g\_{i}^{∘}+RT\sum\_{i=1}^{c}n\_{i}lnX\_{i}+G^{ex}$ (C.1)

where

$G^{ex}=RT\left[\sum\_{i=1}^{c}n\_{ii}ln\left(\frac{X\_{ii}}{Y\_{i}^{2}}\right)+\sum\_{i=1}^{c−1}\sum\_{\begin{matrix}j=2\\j>i\end{matrix}}^{c}n\_{ij}ln\left(\frac{X\_{ij}}{2Y\_{i}Y\_{j}}\right)\right]+\sum\_{i=1}^{c−1}\sum\_{\begin{matrix}j=2\\j>i\end{matrix}}^{c}\frac{n\_{ij}}{2}Δg\_{ij}$ (C.2)

Through the same procedure introduced in **section [4](#sec_model)**, $γ\_{M}$ and $γ\_{O}$ are then obtained using Eq. (15):

$\begin{matrix}ln γ\_{M}&=&\frac{Z}{2}\left[ln\frac{1−2X\_{O}}{\left(1−X\_{O}\right)^{2}}+\frac{2X\_{O}^{2}}{1−X\_{O}}+\frac{2X\_{O}}{Q^{2}}\left(\sum\_{k=1}^{c−1}K\_{kO}X\_{k}\left(K\_{MO}ln\left(\frac{K\_{MO}}{K\_{kO}}\right)+Q−K\_{MO}\right)\right)\right]\\&+&\frac{Z}{2RT}\left[\begin{array}{c}\frac{3X\_{O}−1}{\left(1−X\_{O}\right)^{3}}\sum\_{\begin{matrix}j=2\\j>i\end{matrix}}^{c−1}\sum\_{i=1}^{c−2}X\_{i}X\_{j}Δg\_{ij}+\frac{1−2X\_{O}}{\left(1−X\_{O}\right)^{2}}\sum\_{\begin{matrix}k=1\\k\ne M\end{matrix}}^{c−1}X\_{k}Δg\_{kM}\\+\frac{K\_{MO}X\_{O}}{Q^{2}}\sum\_{k=1}^{c−1}K\_{kO}X\_{k}\left(Δg\_{MO}−Δg\_{kO}\right)\end{array}\right]\\&&\end{matrix}$ (C.3)

and

$\begin{matrix}ln γ\_{O}&=&\frac{Z}{2}\left[ln\frac{\left(1−X\_{O}\right)^{2}}{1−2X\_{O}}+\sum\_{k=1}^{c−1}\frac{K\_{kO}X\_{k}}{Q}ln\frac{K\_{kO}}{Q}\right]\\&+&\frac{Z}{2RT}\left[\sum\_{k=1}^{c−1}\frac{K\_{kO}X\_{k}}{Q}Δg\_{kO}−\frac{1}{\left(1−X\_{O}\right)^{2}}\sum\_{\begin{matrix}j=2\\j>i\end{matrix}}^{c−1}\sum\_{i=1}^{c−2}X\_{i}X\_{j}Δg\_{ij}\right]\end{matrix}$ (C.4)

where

$Q=\sum\_{k=1}^{c−1}K\_{kO}X\_{k}=\sum\_{k=1}^{c−1}exp\left(−\frac{Δg\_{kO}−Δg\_{FeO}}{2RT}\right)X\_{k}$ (C.5)

with $K\_{kO}=1$ when $k=1$ (Fe). For example, $Q$ in a liquid steel composed of Fe–C–Si–Mn–Al–O is computed as follows:

$Q=X\_{Fe}+K\_{CO}X\_{C}+K\_{SiO}X\_{Si}+K\_{MnO}X\_{Mn}+K\_{AlO}X\_{Al}$ (C.6)

where

$K\_{CO}= exp\left(−\frac{Δg\_{CO}−Δg\_{FeO}}{2RT}\right)$ (C.7)

$K\_{SiO}= exp\left(−\frac{Δg\_{SiO}−Δg\_{FeO}}{2RT}\right)$ (C.8)

$K\_{MnO}= exp\left(−\frac{Δg\_{MnO}−Δg\_{FeO}}{2RT}\right)$ (C.9)

$K\_{AlO}= exp\left(−\frac{Δg\_{AlO}−Δg\_{FeO}}{2RT}\right)$ (C.10)

Eqs. (C.3) and (C.4) are reduced to Eqs. (49) and (50), respectively, when $c$ = 3.

Eqs. (C.3) and (C.4) provide explicit functions of composition and temperature for $γ\_{M}$ and $γ\_{O}$, respectively. Thus, $γ\_{M}$ and $γ\_{O}$ can be directly calculated without internal Gibbs energy minimization when the composition and temperature of the system are known. This computational approach eliminates the additional step of internal equilibrium calculation (Fig. [1](#fig_20)).

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