Appendix A – Terms of the energy balance in the elaboration zone

This appendix presents the calculation methodology for the energy balance of Eq.(37). The **Table 6** gathers the equations for the calculation of the different q as a function of the temperature of the corresponding stream j (T_j) and the temperature of the thermal reserve zone (T_R). In his original work, Rist only provided data for $T_R = 1000$ °C and fixed values of T_j. Furthermore, we work in kcal per mole of Fe, as Rist did in his original work, to facilitate comparison [10].

The calculation of the y variables is given as a function of the mass flows of the corresponding stream, m_j, and the mass fraction of each compound i in that stream, $\Omega_{j,i}$. When solving the Rist diagram, we assume that the mass and composition of Iron ore, Pulverized coal, Injectants and Hot metal are known (**Figure 4**). The moisture in the air is also fixed.

It must be noted that to obtain the coordinates X_P and Y_P we actually need to compute Eq.(39), Eq.(40), Eq.(41) and Eq.(43), instead of Eq.(37). For this reason, the terms y_v and y_d are not computed. These two variables are results from the model, not inputs.

A.1 Term $q_c y_v$: heat released by the incomplete combustion of carbon

The heat released by the incomplete combustion of carbon with the air at the tuyeres (per mol of Fe in the hot metal) is denoted by $q_c y_v$. The term is given as a function of the moles of O entering with the air, so it may account for any carbon independently of the source (coke or injectants). The fact that it can account for the carbon of different sources does not imply that it accounts for the incomplete combustion of all of the carbon. Some part of the carbon will be partially combusted by using the O from the injectants itself (e.g., O contained in pulverized coal) instead of with O from air. That part is accounted in the corresponding term $q_j y_j$ of each injectant.

The variable q_c is the heat released through the reaction of Eq.(16). Thermodynamic data for carbon is usually provided for graphite. However, we have part of the carbon coming from coke. Therefore, the enthalpy change in the graphitization of coke carbon must be taken into account Eq.(63) [11]. Since we do not know how much carbon comes from coke and how much from the decomposition of the injectants (and it will be different for each configuration), we make the calculations considering all carbon as coke carbon (Eq.(64)). Therefore, we will have to consider that injectants decompose into coke carbon, instead of graphite, when computing $q_j y_j$.

$$\text{C (coke)} \rightarrow \text{C (graphite)} \qquad \Delta H = -5.02\ \text{kJ/mol} \tag{63}$$

$$\text{C (coke)} + 0.5\ \text{O}_2 \rightarrow \text{CO} \qquad \Delta H = -118.7\ \text{kJ/mol} \tag{64}$$

The heat released by the incomplete combustion of coke carbon (Eq.(65)) was tabulated using data from NIST and Aspen Plus data bases as a function of temperature. These data were adjusted to a polynomial of degree 5 (Eq.(113), **Table 6**). The temperature at which q_c must be calculated is T_R, i.e., the temperature of the thermal reserve zone.

$$q_c = h_{\text{C(coke)}} + 0.5\ h_{\text{O2}} - h_{\text{CO}} \tag{65}$$

The variable y_v is unknown and is calculated as a result from the operating line (computed from the intercept Y_E).

A.2 Term $q_v y_v$: sensible heat of the air

The air is injected in the blast furnace at temperatures higher than T_R. Since we select T_R as the reference temperature for the energy balance, it means that the air will provide its sensible heat between T_v and T_R as available heat (left side of Eq.(37)). The term $q_v y_v$ denotes this energy. For its calculation, we tabulated data of $c_{p,air}$ and adjusted it to a polynomial of degree 3. Then, we integrated that equation (Eq.(66)), thus obtaining Eq.(114). To change the units from kcal/mol$_{\text{air}}$ (tabulated data) to kcal/mol$_{\text{O}}$, (our model units) the factor 0.42 mol$_{\text{O}}$/mol$_{\text{air}}$ is used.

$$q_v = \int_{T_R}^{T} c_{p,air}\, dT \tag{66}$$

The variable y_v is unknown and is calculated as a result from the operating line (computed from the intercept Y_E).

A.3 Term $q_{iw} Y_w$: heat released by the reduction of wüstite

The term $q_{iw} Y_w$ denotes the heat released by the reduction of wüstite to iron, per mol of Fe produced in the blast furnace. Three assumptions are taken for this term:

- Only wüstite is entering the middle zone (i.e., ideal operation, with operating line passing through point W). This assumption is corrected later with the term δ.
- The reduction of wüstite takes place only through indirect reduction. This is corrected with the heat absorbed during direct reduction (term $q_g y_d$).
- All the reduction is carried out by CO (Eq.(5)). This is corrected through q_k, which appears in different terms referring to hydrogen. The term q_k accounts for the energy absorbed during the reverse water-gas shift reaction. In other words, the reverse of Eq.(7) plus Eq.(5) is equal to Eq.(6).

The variable Y_w is known (see **Table 1**), denoting the number of moles of O per mol of Fe in wüstite. The variable q_{iw} is tabulated as a function of temperature with data from NIST and Aspen Plus data bases (Eq.(67)). It must be mentioned that the computed values differ between the two databases. The data from Aspen was chosen for the data fit of Eq.(113) (**Table 6**).

$$q_{iw} = h_{\mathrm{Fe_{0.95}O}} + h_{\mathrm{CO}} - 0.95\, h_{\mathrm{Fe}} - h_{\mathrm{CO2}} \tag{67}$$

In the energy balance, q_{iw} must be calculated at T_R.

A.4 Term δ: lack of chemical ideality in wüstite reduction

The term δ is used to correct $q_{iw}Y_w$, since it assumed that only wüstite is entering the middle zone (which is not the case under non-ideal conditions). The presence of magnetite in the elaboration zone makes the available heat to decrease because the reduction of magnetite to wüstite is endothermic (Eq.(3)). Assuming a mixture of wüstite and magnetite characterized by Y_R, the term δ is given by Eq.(68). This equation is a simplification for $Fe_{0.95}O$-Fe_3O_4 mixtures derived from a triangular diagram for Fe-$Fe_{0.95}O$-Fe_3O_4 mixtures (see annexes of [11]).

$$\delta = (Y_R - 1.05) \cdot (3.75 \cdot q_{iw} - 4.75 \cdot q_{im}) \tag{68}$$

The term q_{im} is the heat released by the overall reaction Eq.(69) (for the energy balance, q_{im} must be calculated at T_R). To compute it in kcal/mol_O, it is used Eq.(70). It must be mentioned that the computed values for q_{im} differ between different databases (Aspen Plus and NIST). The data from Aspen was chosen for the data fit of Eq.(113) (**Table 6**).

$$\mathrm{Fe_3O_4} + 4\ \mathrm{CO} \rightarrow 3\ \mathrm{Fe} + 4\ \mathrm{CO_2} \tag{69}$$
$$q_{im} = 0.25\, h_{\mathrm{Fe_3O_4}} + h_{\mathrm{CO}} - 0.75\, h_{\mathrm{Fe}} - h_{\mathrm{CO2}} \tag{70}$$

As occurred for $q_{iw}Y_w$, the variable δ assumes that reduction takes place only by CO. The energy that would be consumed by the H_2 during the reduction is accounted in those terms including q_k.

A.5 Term $q_g(y_d - y_e)$: heat absorbed during direct reduction

The direct reduction of wüstite it is actually the combination of CO_2 (or H_2O) dissociation and the indirect reduction of FeO by CO (or H_2). In the term $q_{iw}Y_w$ it was already accounted the heat released by the indirect reduction, including the comprised during the overall process of direct reduction (because it was computed for all the O atoms in wüstite, i.e., Y_w). It means that here, in the term $q_g(y_d - y_e)$, we have to take into consideration only the heat absorbed because of the CO_2 dissociation. Moreover, not all the O atoms that are reduced from FeO through direct reduction are due to CO_2 dissociation. Some of them will be removed because of the H_2O dissociation. The latter are accounted in the term $q_e y_e$. For this reason, we subtract the moles of O removed because of water dissociation (y_e) to the total moles of O removed during direct reduction (y_d). Thus, the term $q_g(y_d - y_e)$ accounts only for the heat absorbed during the direct reduction of wüstite when it occurs through Eq.(9).

It must be noted that this correction was not made by Rist in his original work. He considered that all the O atoms removed by direct reduction were because of the CO_2 dissociation and, in addition, he accounted for the H_2O dissociation of the hot blast. Therefore, he overestimates the absorbed heat by direct reduction, because he accounted the absorbed heat twice for a number of moles equals to y_e (once through CO_2 dissociation and again through H_2O dissociation).

To know the term $q_g(y_d - y_e)$ we would have to compute the variables q_g, y_d, and y_e. Nevertheless, when calculating X_P and Y_P, which is what we want, there is no need to compute y_d. Actually, the variable y_d will be a result from the operating line (Eq.(55)). Regarding y_e, it is written as $y_e = e y_v$ during the construction of Eq.(38), where e is the moisture of the hot blast in mol_{H2O}/mol_O, calculated by Eq.(71) as a function of air humidity, η (assumed known, in g/Nm^3) . Again, we do not need y_v, which will be a result from the operating line (Eq.(52)).

$$e = \eta/(18.75 \mathrm{M_{H2O}}) \tag{71}$$

Lastly, the variable q_g is the heat absorbed by the CO_2 dissociation, calculated as Eq.(72) at T_R and tabulated in **Table 6**.

$$q_g = 2h_{\mathrm{CO}} - h_{\mathrm{C(coke)}} - h_{\mathrm{CO_2}} \tag{72}$$

It must be noted that per 1 mol of O reduced from iron by Eq.(8), only 1 mol of C is consumed in Eq.(9). For this reason, there is no problem in mixing the units kcal/mol_C of q_g and the units mol_O/mol_{Fe} of y_d in the term $q_g y_d$, since mol_C and mol_O are equivalent in this case. The same occurs with the dissociation of H_2O and the units of y_e.

A.6 Term $q_k y_k$: heat consumed due to the hydrogen entering with the coke

The term $q_k y_k$ is the heat consumed by the hydrogen entering with the coke because of the reverse water-gas shift reaction. The variable y_k is the number of moles of H_2 in the coke per mole of Fe produced (Eq. (73)). This is written as a function of the coke mass flow rate and its H mass fraction, which are assumed known. The number of moles of Fe produced are calculated by Eq.(74) as a function of the Fe mass fraction in the hot metal (also assumed known).

$$y_k = 10^3 \Omega_{\mathrm{K,H}} \mathrm{m_K}/(\mathrm{M_{H2}} n_{\mathrm{HM,Fe}}) \tag{73}$$

$$n_{\mathrm{HM,Fe}} = \Omega_{\mathrm{HM,Fe}} 10^6/\mathrm{M_{Fe}} \tag{74}$$

Regarding q_k, it stands for the heat consumed per mole of H_2 in the reducing gas (whether the mole react or not, kcal/mol$_{H2}$). In order to write this heat, it is used the Eq.(75). It comprises ω_{WH} and q_ε. The former is the number of H_2 moles that has reacted (by the moment the gas reaches the thermal reserve zone) per moles of H_2 that were in the reducing gas at the beginning, i.e., ω_{WH} (Eq.(32), **Table 2**, calculated at T_R). In other words, it must be understood as the fraction of H_2 that reacts inside the control volume (mol$_{H2(reacting)}$/mol$_{H2}$). The other variable, q_ε, is the heat absorbed by the reverse water-gas shift, calculated through Eq.(76), whose units are kcal/mol$_{H2(reacting)}$ (tabulated in **Table 6**).

$$q_k = \omega_{WH} q_\varepsilon \tag{75}$$

$$q_\varepsilon = h_{\mathrm{H_2O}} + h_{\mathrm{CO}} - h_{\mathrm{H_2}} - h_{\mathrm{CO_2}} \tag{76}$$

The term q_k will appear also in all other terms related to hydrogen. Thanks to this, other terms like $(q_{iw}Y_w - \delta)$ can be written as a function of CO only, because the endothermic behavior of H_2 has been considered in advance in q_k. In other words, Eq.(6) is equivalent to Eq.(5) plus the reverse of Eq.(7) for example.

A.7 Term $q_e y_e$: overall heat absorbed by the moisture of the air

The term $q_e y_e$ represents the overall heat that is absorbed because of the presence of moisture in the air. The variable q_e (Eq.(77)) has three contributions that comprise the dissociation of H_2O during the direct reduction of wüstite (q_{er}), the endothermic behavior during indirect reduction (q_k), and the sensible heat (q_{es}).

$$q_e = q_{er} + q_k + q_{es} \tag{77}$$

The meaning of variable q_k was explained in detail in Appendix A.6 (Eq.(75)) and it is used to correct the assumption taken in $q_{iw}\mathrm{Y_w}$ (Appendix A.3) for which all the reduction of wüstite occurred by CO (which is not true). The variable q_{es} is the sensible heat of the water in the air between its inlet temperature T_v and the temperature of the thermal reserve zone T_R. Since it appears in the right side of Eq.(37) as a sink of heat, instead of as a contribution, it was calculated by Eq.(78) (tabulated in **Table 6** in the form of Eq.(114) with $T = T_v$).

$$q_{es} = -\int_{T_R}^{T} c_{p,\mathrm{H_2O}}\, dT \tag{78}$$

Lastly, the variable q_{er} standing for the heat absorbed during H_2O dissociation (which takes place at the tuyeres and it forms part of the overall direct reduction process) is calculated by Eq.(79) (also tabulated in **Table 6**).

$$q_{er} = h_{\mathrm{CO}} + h_{\mathrm{H2}} - h_{\mathrm{C(coke)}} - h_{\mathrm{H_2O}} \tag{79}$$

The variable y_e denotes the number of moles of H_2O in hot blast. This is written as $y_e = e y_v$, where e is given by Eq.(71) as a function of air humidity (assumed known) and y_v is computed by Eq.(52) as a result from the operating line (not needed for the calculation of point P).

A.8 Term $\sum q_j y_j$: overall heat absorbed by the injection of auxiliary fuels

The summation $\sum q_j y_j$ stands for all the injections in the tuyeres (except for the hot blast). Each addend $q_j y_j$ corresponds to one single injection, which might be an auxiliary reducing agent (pulverized coal, natural gas, hydrogen, etc.) or an injection of oxygen to enrich the blast. Thus, we may have injections with an overall chemical formula $\mathrm{CH_{2a}O_{2b}N_{2c}S_{2d}Z_z}$, $\mathrm{H_{2a}O_{2b}N_{2c}}$ or even $\mathrm{O_{2b}N_{2c}}$. The term y_j is the number of moles injected (mol$_{\mathrm{CH_{2a}O_{2b}N_{2c}S_{2d}Z_z}}$, mol$_{\mathrm{H_{2a}O_{2b}N_{2c}}}$ or mol$_{\mathrm{O_{2b}N_{2c}}}$) per mole of Fe in the hot metal, calculated by Eq.(80) (the mass m_j is assumed known). The molar weight is calculated using Eq.(81), and the parameters a, b, c, d, z by using Eq.(82) to Eq.(86) (for the gas injections, we only consider CO, CO_2, H_2, H_2O, CH_4, O_2 and N_2 as potential constituents of the gas; their molar fractions in the gas injected are assumed known $\omega_{j,\mathrm{i}}$). The notation z_i refers to each of the components of the ashes in coal (see Appendix B for more detail).

$$y_j = 10^3\, \mathrm{m}_j/(\mathrm{M_j} n_{\mathrm{HM,Fe}}) \tag{80}$$

$$M_j = \begin{cases} M_C + aM_{H_2} + bM_{O_2} + cM_{N_2} + dM_{S_2} + \sum_i z_i M_{Z_i} & \text{for } \mathrm{CH_{2a}O_{2b}N_{2c}S_{2d}Z_z} \\ aM_{H_2} + bM_{O_2} + cM_{N_2} & \text{for } \mathrm{H_{2a}O_{2b}N_{2c}} \ or\ \mathrm{O_{2b}N_{2c}} \end{cases} \tag{81}$$

$$a = \begin{cases} \dfrac{\left(\Omega^{d}_{\mathrm{j,H}}(1-\Omega_{\mathrm{j,M}}) + \Omega_{\mathrm{j,M}}\dfrac{\mathrm{M_{H_2}}}{\mathrm{M_{H_2O}}}\right)/\mathrm{M_{H_2}}}{\Omega^{d}_{\mathrm{j,C}}\left(1-\Omega_{\mathrm{j,M}}\right)/\mathrm{M_C}} & \text{for coal or biomass } (\mathrm{CH_{2a}O_{2b}N_{2c}S_{2d}Z_z}) \\ \dfrac{2\omega_{j,\mathrm{CH4}} + \omega_{j,\mathrm{H2}} + \omega_{j,\mathrm{H2O}}}{\omega_{j,\mathrm{CH4}} + \omega_{j,\mathrm{CO}} + \omega_{j,\mathrm{CO2}}} & \text{for gas } (\mathrm{CH_{2a}O_{2b}N_{2c}S_{2d}Z_z}) \\ \dfrac{\omega_{j,\mathrm{H2}} + \omega_{j,\mathrm{H2O}}}{\omega_{j,\mathrm{O2}} + 0.5\omega_{j,\mathrm{H2O}}} & \text{for gas } (\mathrm{H_{2a}O_{2b}N_{2c}}) \\ 0 & \text{for gas } (\mathrm{O_{2b}N_{2c}}) \end{cases} \tag{82}$$

$$b = \begin{cases} \dfrac{\left(\Omega^{d}_{\mathrm{j,O}}(1-\Omega_{\mathrm{j,M}}) + \Omega_{\mathrm{j,M}}\dfrac{\mathrm{M_{O}}}{\mathrm{M_{H_2O}}}\right)/\mathrm{M_{O_2}}}{\Omega^{d}_{\mathrm{j,C}}\left(1-\Omega_{\mathrm{j,M}}\right)/\mathrm{M_C}} & \text{for coal or biomass } (\mathrm{CH_{2a}O_{2b}N_{2c}S_{2d}Z_z}) \\ \dfrac{0.5\omega_{j,\mathrm{CO}} + \omega_{j,\mathrm{CO2}} + 0.5\omega_{j,\mathrm{H2O}} + \omega_{j,\mathrm{O2}}}{\omega_{j,\mathrm{CH4}} + \omega_{j,\mathrm{CO}} + \omega_{j,\mathrm{CO2}}} & \text{for gas } (\mathrm{CH_{2a}O_{2b}N_{2c}S_{2d}Z_z}) \\ 1 & \text{for gas } (\mathrm{H_{2a}O_{2b}N_{2c}}) \\ 1 & \text{for gas } (\mathrm{O_{2b}N_{2c}}) \end{cases} \tag{83}$$

$$c = \begin{cases} \dfrac{\Omega^{d}_{\mathrm{j,N}}/\mathrm{M_{N_2}}}{\Omega^{d}_{\mathrm{j,C}}/\mathrm{M_C}} & \text{for coal or biomass } (\mathrm{CH_{2a}O_{2b}N_{2c}S_{2d}Z_z}) \\ \dfrac{\omega_{j,\mathrm{N2}}}{\omega_{j,\mathrm{CH4}} + \omega_{j,\mathrm{CO}} + \omega_{j,\mathrm{CO2}}} & \text{for gas } (\mathrm{CH_{2a}O_{2b}N_{2c}S_{2d}Z_z}) \\ \dfrac{\omega_{j,\mathrm{N2}}}{\omega_{j,\mathrm{O2}} + 0.5\omega_{j,\mathrm{H2O}}} & \text{for gas } (\mathrm{H_{2a}O_{2b}N_{2c}}) \\ \dfrac{\omega_{j,\mathrm{N2}}}{\omega_{j,\mathrm{O2}}} & \text{for gas } (\mathrm{O_{2b}N_{2c}}) \end{cases} \tag{84}$$

$$d = \frac{\Omega^{d}_{\mathrm{j,S}}/\mathrm{M_{S_2}}}{\Omega^{d}_{\mathrm{j,C}}/\mathrm{M_C}} \tag{85}$$

$$z_i = \frac{\Omega^{d}_{\mathrm{j,Z_i}}/\mathrm{M_{Z_i}}}{\Omega^{d}_{\mathrm{j,C}}/\mathrm{M_C}} \tag{86}$$

Then, the thermal demand q_j (Eq.(87)) covers the dissociation of the injection (q_{jd}), its sensible heat (q_{js}), the endothermal behavior of H_2 during indirect reduction ($a\ q_k$), the utilization of the O_2 for combustion ($-2b\ q_c$), and the transfer of S to the slag ($-2d\ q_S$).

$$q_j = q_{jd} + q_{js} + a\ q_k - 2b\ q_c - 2d \cdot q_S \tag{87}$$

The heat of decomposition of the injectant, q_{jd}, must be calculated for each particular case. In the case of gas mixtures of CO, CO_2, H_2, H_2O, CH_4, O_2 and N_2, the heat of decomposition can be conventionally calculated as the enthalpy difference between the products and the reactants in the reaction given by Eq.(88), at T_j. We use the Eq.(89) for this calculation, which is a pondered summation of the components that will decompose (the heats of decomposition of CO, CO_2, CH_4 and H_2O are tabulated in **Table 6**). However, in the case of coal or biomass, the enthalpy is usually unknown because the molecular structure of the solid fuel is unknown. For these cases, a more complex methodology must be followed (please see the Appendix B for the calculation of q_{jd} in the case of coal and biomass).

$$\mathrm{CH_{2a}O_{2b}N_{2c}} \rightarrow \mathrm{C} + \mathrm{aH_2} + \mathrm{bO_2} + \mathrm{cN_2} \tag{88}$$

$$q_{jd} = \begin{cases} \dfrac{\omega_{j,\mathrm{CO}}q_{\mathrm{CO},d} + \omega_{j,\mathrm{CO2}}q_{\mathrm{CO2},d} + \omega_{j,\mathrm{CH4}}q_{\mathrm{CH4},d} + \omega_{j,\mathrm{H2O}}q_{\mathrm{H2O},d}}{\omega_{j,\mathrm{CO}} + \omega_{j,\mathrm{CO2}} + \omega_{j,\mathrm{CH4}}} & \text{for gas } (\mathrm{CH_{2a}O_{2b}N_{2c}S_{2d}Z_z}) \\ \dfrac{\omega_{j,\mathrm{H2O}}q_{\mathrm{H2O},d}}{\omega_{j,\mathrm{O2}} + 0.5\omega_{j,\mathrm{H2O}}} & \text{for gas } (\mathrm{H_{2a}O_{2b}N_{2c}}) \\ 0 & \text{for gas } (\mathrm{O_{2b}N_{2c}}) \end{cases} \tag{89}$$

The sensible heat q_{js} accounts for the heating from T_j to T_R of the products of the decomposition. It is calculated by Eq.(90), where $q_{js,i}$ is the sensible heat of element i (**Table 6**). For the case of coal or biomass, an overall sensible heat of ashes can be used as simplification ($q_{js,\mathrm{Z}}$, given in **Table 6**) with $M_Z = \Omega^{d}_{\mathrm{j,Z}}\left(1-\Omega_{\mathrm{j,M}}\right)M_j/z$ given in g_Z/mol_Z, and $z = \sum z_i$.

$$q_{js} = \begin{cases} q_{js,\mathrm{C}} + aq_{js,\mathrm{H2}} + bq_{js,\mathrm{O2}} + cq_{js,\mathrm{N2}} + dq_{js,\mathrm{S2}} + \mathrm{z}q_{js,\mathrm{Z}} & \text{for } \mathrm{CH_{2a}O_{2b}N_{2c}S_{2d}Z_z} \\ aq_{js,\mathrm{H2}} + bq_{js,\mathrm{O2}} + cq_{js,\mathrm{N2}} & \text{for } \mathrm{H_{2a}O_{2b}N_{2c}} \text{ or } \mathrm{O_{2b}N_{2c}} \end{cases} \tag{90}$$

The two following addends in Eq.(87) (i.e., $+a\ q_k$ and $-2b\ q_c$) are easily calculated with Eq.(82) and Eq.(83) for a and b, with Eq.(75) for q_k, and with **Table 6** for q_c. The last term, $-2d \cdot q_S$, uses the heat released during the transfer of S to the slag (Eq.(18) plus Eq.(19)), calculated by Eq.(91) and tabulated in **Table 6**.

$$q_S = h_{\mathrm{C(coke)}} + h_{\mathrm{CaO}} + 0.5h_{\mathrm{S2}} - h_{\mathrm{CO}} - h_{\mathrm{CaS}} \tag{91}$$

A.9 Term δ': lack of chemical ideality in the conversion of H_2 to H_2O

The variable q_k, which takes account for the H_2 that is converted to H_2O (see Appendix A.6, Eq.(75)), assumed that the reacted amount corresponds to the equilibrium of the H-O-Fe system at T_R (i.e., the fraction of H_2 that reacted is given by ω_{WH}). However, this would be the case only under an ideal situation in which all the exchangeable oxygen is exchanged (i.e., chemical efficiency $r = 1$), which in practice will not be the case. To take into account that less H_2 has been converted to H_2O than would correspond to an ideal case (i.e., we are at point R instead of W), the heat absorbed by the reverse water-gas shift reaction is corrected in all terms where q_k appears. The correction is written as Eq.(92), thus diminishing the contribution of q_k in Eq.(37) by a fraction $(1 - r)$.

$$\delta' = (1 - r)\left(y_k + y_e + \sum a_j y_j\right) q_k \tag{92}$$

The chemical efficiency r is assumed known, and the calculation of the other involved variables has been explained in other appendixes (Appendix A.5 for y_e, Appendix A.6 for y_k, q_k, and Appendix A.8 for $a_j y_j$).

A.10 Terms $q_{\mathrm{Si}}y_{\mathrm{Si}}$, $q_{\mathrm{Mn}}y_{\mathrm{Mn}}$ and $q_P y_P$: heat absorbed by the reduction of the accompanying elements

The heat consumed during the reduction of the accompanying elements is accounted by the terms $q_{\mathrm{Si}}y_{\mathrm{Si}}$, $q_{\mathrm{Mn}}y_{\mathrm{Mn}}$ and $q_{\mathrm{P}}y_{\mathrm{P}}$. The variables q_{Si}, q_{Mn} and q_{P} correspond to the heat of reactions of Eq.(11), Eq.(12) and Eq.(13), respectively, but calculated in kcal/mol$_{\mathrm{CO}}$ (equivalent to kcal/mol$_{\mathrm{O}}$, because 1 mole of O gives 1 mole of CO). Thus, they are computed by Eq.(93), Eq.(94) and Eq.(95), and tabulated in **Table 6**. For the energy balance of the operating line, these must be calculated at T_R.

$$q_{\mathrm{Si}} = h_{\mathrm{CO}} + 0.5h_{\mathrm{Fe_3Si}} - h_{\mathrm{C(coke)}} - 0.5h_{\mathrm{SiO_2}} - 1.5h_{\mathrm{Fe}} \tag{93}$$
$$q_{\mathrm{Mn}} = h_{\mathrm{CO}} + h_{\mathrm{Mn}} - h_{\mathrm{C(coke)}} - h_{\mathrm{MnO}} \tag{94}$$
$$q_{\mathrm{P}} = h_{\mathrm{CO}} + 0.6h_{\mathrm{CaO}} + 0.4h_{\mathrm{Fe_3P}} - h_{\mathrm{C(coke)}} - 0.2h_{\mathrm{P_2O_5\cdot 3CaO}} - 1.2h_{\mathrm{Fe}} \tag{95}$$

The variables y_{Si}, y_{Mn} and y_{P} are the number of moles of O removed from the accompanying element during its reduction (i.e., the moles of CO generated because of their reduction), per mole of Fe produced in hot metal. They are calculated by Eq.(96), Eq.(97) and Eq.(98) as a function of the mass fractions of Si, Mn and P (assumed known), and the variable $n_{\mathrm{HM,Fe}}$ (Eq.(74), also known). The calculation can be understood as the product of the number of CO moles generated per mole of Si/Mn/P ending up in the hot metal (mol$_{\mathrm{CO}}$/mol$_{\mathrm{i}}$) by the moles of Si/Mn/P in the hot metal per ton of hot metal (mol$_{\mathrm{i}}$/t$_{\mathrm{HM}}$), and divided by the moles of Fe in hot metal per ton of hot metal (mol$_{\mathrm{Fe}}$/t$_{\mathrm{HM}}$). Thus, the three of them have the units mol$_{\mathrm{CO}}$/mol$_{\mathrm{Fe}}$.

$$y_{\mathrm{Si}} = 2(10^6\Omega_{\mathrm{HM,Si}}/\mathrm{M_{Si}})/n_{\mathrm{HM,Fe}} \tag{96}$$
$$y_{\mathrm{Mn}} = (10^6\Omega_{\mathrm{HM,Mn}}/\mathrm{M_{Mn}})/n_{\mathrm{HM,Fe}} \tag{97}$$
$$y_{\mathrm{P}} = 2.5(10^6\Omega_{\mathrm{HM,P}}/\mathrm{M_{P}})/n_{\mathrm{HM,Fe}} \tag{98}$$

A.11 Term $q_\gamma \gamma$: heat absorbed by the carburization of the iron

The term $q_\gamma \gamma$ is the heat consumed during reactions of Eq.(14) and Eq.(15), i.e., during the carburization of iron. Rist used a fixed value for q_γ (4.2 kcal/mol$_{\mathrm{C}}$) in his calculations [10]. Here we provide Eq.(99), where $\gamma_{\gamma\mathrm{Fe}}$ and $\gamma_{\mathrm{Fe_3C}}$ are the number of moles of carbon dissolved in the hot metal as austenite and cementite (mol$_{\mathrm{C}}$/mol$_{\mathrm{Fe}}$) (Eq.(100) and Eq.(101)). As simplification, we can assume that there is 1.5% (in weight) of carbon as austenite in the hot metal ($\Omega_{\mathrm{HM},\gamma\mathrm{Fe}} = 0.015$), and the rest of carbon is cementite ($\Omega_{\mathrm{HM,Fe_3C}} = \Omega_{\mathrm{HM,C}} - \Omega_{\mathrm{HM},\gamma\mathrm{Fe}}$) [11].

$$q_\gamma \gamma = q_{\gamma\mathrm{Fe}} \cdot \gamma_{\gamma\mathrm{Fe}} + q_{\mathrm{Fe_3C}} \cdot \gamma_{\mathrm{Fe_3C}} \tag{99}$$
$$\gamma_{\gamma\mathrm{Fe}} = (10^6\Omega_{\mathrm{HM},\gamma\mathrm{Fe}}/\mathrm{M_C})/n_{\mathrm{HM,Fe}} \tag{100}$$
$$\gamma_{\mathrm{Fe_3C}} = (10^6\ \Omega_{\mathrm{HM,Fe_3C}}/\mathrm{M_C})/n_{\mathrm{HM,Fe}} \tag{101}$$

The terms $q_{\gamma\mathrm{Fe}}$ and $q_{\mathrm{Fe_3C}}$ are the heat absorbed by the corresponding reactions in kcal/mol$_{\mathrm{C}}$ (Eq.(102) and Eq.(103)). The value of $q_{\gamma\mathrm{Fe}}$ is taken from [10].

$$q_{\gamma\mathrm{Fe}} = 8.3\ \mathrm{kcal/mol_C} \tag{102}$$
$$q_{\mathrm{Fe_3C}} = h_{\mathrm{Fe_3C}} - 3h_{\mathrm{Fe}} - h_{\mathrm{C}} \tag{103}$$

The terms $q_{\gamma\mathrm{Fe}}$ and $q_{\mathrm{Fe_3C}}$ are tabulated in **Table 6** according to Eq.(113). It is worth to mention that the value of $q_{\mathrm{Fe_3C}}$ provided here for 1000 °C (3.8 kcal/mol$_{\mathrm{C}}$) differs from the value provided by Rist (1.6 kcal/mol$_{\mathrm{C}}$). We use the Aspen Plus database for this kind of calculation.

A.12 Term f: sensible heat of the hot metal

The sensible heat of the hot metal can be written as summation of the sensible heat of its constituents pondered by their molar fraction [34]. Therefore, we write the term f as Eq.(104), in kcal/mol$_{\text{Fe}}$, where $q_{f,i}$ includes the sensible heat of element i between T_f and T_R, plus its heat of fusion. The variables $\Omega_{\text{HM},\gamma\text{Fe}}$ and $\Omega_{\text{HM,Fe}_3\text{C}}$ are the mass fractions of C in hot metal when dissolved as austenite and cementite respectively, with $\Omega_{\text{HM,C}} = \Omega_{\text{HM},\gamma\text{Fe}} + \Omega_{\text{HM,Fe}_3\text{C}}$.

$$f = \sum_i \frac{\left(\frac{\Omega_{\text{HM,i}}}{\text{M}_\text{i}} q_{f,i}\right)}{\left(\frac{\Omega_{\text{HM,Fe}}}{\text{M}_{\text{Fe}}}\right)} = q_{f,\text{Fe}} + \frac{\text{M}_{\text{Fe}}}{\Omega_{\text{HM,Fe}}}\left(\frac{\Omega_{\text{HM,Si}}}{\text{M}_{\text{Si}}} q_{f,\text{Si}} + \frac{\Omega_{\text{HM,Mn}}}{\text{M}_{\text{Mn}}} q_{f,\text{Mn}} + \frac{\Omega_{\text{HM,P}}}{\text{M}_{\text{P}}} q_{f,\text{P}} + \frac{\Omega_{\text{HM},\gamma\text{Fe}}}{\text{M}_{\text{C}}} q_{f,\gamma\text{Fe}} + \frac{\Omega_{\text{HM,Fe}_3\text{C}}}{\text{M}_{\text{C}}} q_{f,\text{Fe}_3\text{C}}\right) \tag{104}$$

The variables $q_{f,i}$ (Eq.(105)) are adjusted to Eq.(114) using data from Aspen Plus data base and NIST data base (**Table 6**). By direct comparison of Eq.(105) and Eq.(114), it can be seen that the heat of fusion coincides with the term a_0 in that equation, while the integration of c_p between T_f and T_R is calculated by the rest of the terms of Eq.(114).

$$q_{f,i} = \Delta h_{f,i} + \int_{T_R}^{T_f} c_{p,i}\, dT \tag{105}$$

The heat of fusion of carbon, when forming part of austenite and cementite, is calculated using data taken from [35]. The heat of fusion of pure austenite is 59.29 cal/g, which corresponds to 53.69 kcal/mol$_{\text{Fe16C}}$ (the Fe atoms of austenite forming a face centered cubic crystal structure, and one C atom in the middle of an edge). The contribution of C to this heat of fusion is 1/17, thus obtaining 3.16 kcal/mol$_{\text{C(austenite)}}$. The same reasoning is follow for cementite, whose heat of fusion is 64.93 cal/g, corresponding to 11.66 kcal/mol$_{\text{Fe3C}}$. The contribution of C to this heat of fusion is 1/4, i.e., 2.91 kcal/mol$_{\text{C(cementite)}}$.
Rist, in his original work, only provided a simple overall formula as a function of the exit temperature of the hot metal (Eq.(106)) [11]. This formula is only valid for $T_R = 1000$ °C and the hot metal composition he used in his studies ($\Omega_{\text{HM,Fe}} = 0.937$, $\Omega_{\text{HM,Si}} = 0.004$, $\Omega_{\text{HM,Mn}} = 0.003$, $\Omega_{\text{HM,P}} = 0.018$, $\Omega_{\text{HM},\gamma\text{Fe}} = 0.015$ and $\Omega_{\text{HM,Fe}_3\text{C}} = 0.023$). If we compare results of Eq.(104) for this particular case to the results of Eq.(106), we found they match well with an error below 5% (**Figure 9**). Therefore, we can consider that the general formula we provided is validated.

$$f_{(\text{Rist})} = 9.8349 \cdot 10^{-3}\, T_f - 5.6625 \tag{106}$$

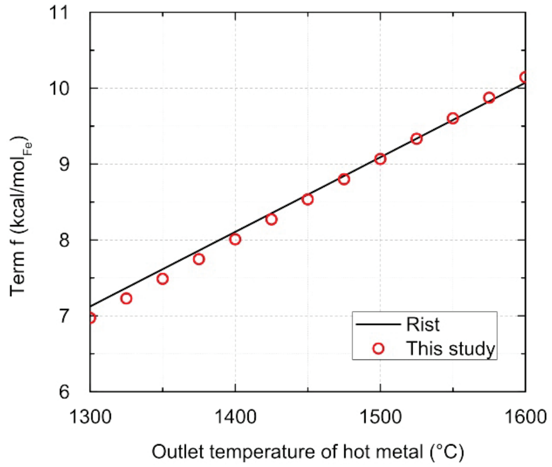

Figure 9. Comparison of term f (kcal/mol$_{\text{Fe}}$) vs. the exit temperature of the hot metal, calculated through the general formula elaborated in this study and through the overall formula provided by Rist, for a particular hot metal composition ($\Omega_{HM,Fe} = 0.937$, $\Omega_{HM,Si} = 0.004$, $\Omega_{HM,Mn} = 0.003$, $\Omega_{HM,P} = 0.018$, $\Omega_{HM,\gamma Fe} = 0.015$ and $\Omega_{HM,Fe_3C} = 0.023$) and $T_R = 1000\ °C$.

We have shown here that the term f does not account in any way for the sensible heat of the slag of for its heat of fusion. It is important to notice this because Rist assumed that Eq.(106) do account for the slag, when it is clearly not the case. Therefore, he remarkably underestimated the necessary heat inside the furnace and, as a consequence, the required amount of coke. Fortunately for Rist, this error was partially counterbalanced by the overestimation he made of the heat absorbed by direct reduction (explained in Appendix A.5). Even so, the final coke amount calculated by Rist is still lower than it should be because his underestimation of the energy for slag heating and melting (about 40% less heat than actually required) is bigger than the overestimation of the heat consumed by direct reduction (34% greater than actually consumed).

A.13 Term l: sensible heat of the slag

The sensible heat of the slag is the summation of the sensible heat of its constituents [34]. Since in this case we do not know the final composition of the slag, we have to calculate this value as a function of the inlets. We write the term l as Eq.(107), in kcal/mol$_{Fe}$, where the term $\left(10^3\Omega_{j,i}m_j\right)/\left(M_i\ n_{HM,Fe}\right)$ is the number of moles of element i (SiO_2, Al_2O_3, CaO, MgO) coming from the iron source j (iron ore, coke, coal) per mole of Fe in hot metal (with $n_{HM,Fe}$ given by (74)). The term $q_{l,i}$ is the sensible heat of compound i between T_l and T_R plus its heat of fusion (Eq.(108), which is adjusted to Eq.(114) and tabulated in **Table 6**). Additionally, the contribution of SiO_2 has to be diminished according to the moles of Si that end up dissolved in the hot metal (term 0.5 $q_{l,SiO_2}y_{Si}$, with y_{Si} given by Eq.(96)). It should be noted that we neglect minor components in the slag as simplification, so the index of summation i only covers SiO_2, Al_2O_3, CaO and MgO.

$$l = \sum_j \sum_i \left(\frac{10^3\Omega_{j,i}m_j}{M_i\ n_{HM,Fe}}\ q_{l,i}\right) - 0.5\ q_{l,SiO_2}y_{Si} \tag{107}$$

$$q_{l,i} = \Delta h_{f,i} + \int_{T_R}^{T_l} c_{p,i}\, dT \tag{108}$$

While computing the operating line, we assume known all the variables in Eq. (107) except for the mass of coke entering the blast furnace (m_K). In case of solving the entire Rist diagram through an equation solver software, there is no problem because the mass of coke will be given by Eq.(49) when the entire system of equations is solved at once. In case of solving one equation at a time, then we would have to assume a given amount of coke at first (e.g., 300-400 kg), solve the operating line (Eq.(33) and Eq.(34)), compute y_v (Eq.(52)), calculate the actual mass of coke (Eq.(49)), and repeat the calculations with this new value in an iterative process until the assumed value and the calculated value are the same.

Rist, in his original work, only provided a very simplified equation for the calculation of this term (Eq.(109)) [11]. Moreover, his equation is only valid to compute the sensible heat between the outlet temperature of the slag and the outlet temperature of the hot metal, providing that the latter is 1400 °C. He presented the equation in this way because he assumed that f already accounted for the sensible heat of the slag between T_f and T_R, which is actually not the case, as we have shown during the construction of the detailed equation for f (see Appendix A.12).

$$l_{(Rist)} = 2.98034 \cdot 10^{-2}\ T_l - 31.8889 \tag{109}$$

When comparing Eq.(109) to our Eq.(107) (computing in our case the integral of $q_{l,i}$ between T_l and T_f for a fair comparison), we found an additional error in the equation provided by Rist. It seems that Eq.(109) was elaborated using the heat capacity of SiO_2 in kJ/mol instead of kcal/mol, as it can be seen in **Figure 10**. This figure compares the results of Eq.(109), with the results of Eq.(107) when c_{p,SiO_2} is deliberately taken with the wrong units kJ/mol, and with the results of Eq.(107) with the proper units.

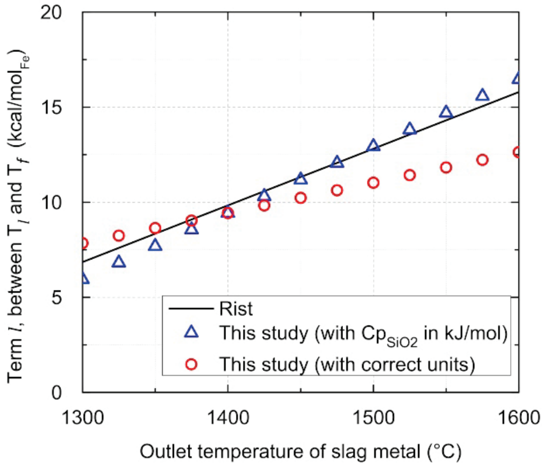

Figure 10. Comparison of term l (kcal/mol$_{Fe}$) vs. the exit temperature of the slag, calculated through the general formula elaborated in this study and through the overall formula provided by Rist, for the case of **Table 3**. For proper comparison, the term l was calculated between T_l and T_f, with $T_f = 1400\ °C$ (instead of between T_l and T_R).

In summary, Rist underestimate the heat required inside the blast furnace because not accounting the heating of slag between T_R and T_f (explained in Appendix A.12), but at the same time he overestimated the heat required because of wrongly computing the term l with c_{p,SiO_2} in wrong units, and also because of considering twice the heat absorbed during direct reduction for a number of moles equals to y_e (explained in Appendix A.5). Thus, these three errors counterbalanced more or less, and Rist was able to reach reasonable results.

A.14 Term p: heat removed by the staves

The term p denotes the heat removed by the staves in the elaboration zone (i.e., in the middle and lower zone). It is calculated by Eq.(110) as a fraction of the total heat removed.

$$p = \theta_{st} \cdot q_{st} / n_{\mathrm{HM,Fe}} \tag{110}$$

The total heat removed is denoted by q_{st}, which is typically between 10^5 and $4.2 \cdot 10^5$ kcal/t$_{\mathrm{HM}}$ [10,17–19]. The fraction of this heat that is removed in the elaboration zone, θ_{st}, is usually between 70 – 80%. Both parameters are assumed known during the calculations. It is worth to mention that θ_{st} remarkably affects to the energy balance in the upper zone (Appendix C) and therefore to the final blast furnace gas composition.

A.15 Term $C_{\Delta T_R}$: lack of thermal ideality

In practice, in the thermal reserve zone, where thermal equilibrium is assumed, a non-zero temperature difference may exist between gas and solids. In this case, T_R is assumed to be the temperature of the gas, which is ΔT_R degrees above the temperature of the solids (i.e., solids are at $T_R - \Delta T_R$) [10]. The temperature difference ΔT_R is assumed known.

Under this situation, the energy balance of Eq.(37) is corrected by the term $C_{\Delta T_R}$, which accounts for the sensible heat of solids between T_R and $T_R - \Delta T_R$ (this effect is also taken into account in the energy balance of the upper zone, Appendix C). The term $C_{\Delta T_R}$ is calculated by Eq.(111), where the first addend accounts for the sensible heat of wüstite, the second for the magnetite (assuming that at point R the excess of O/Fe corresponds to magnetite), and the third addend accounts for the accompanying elements and carbon entering at the top of the blast furnace. In this case, the index of summation j goes through iron ore and coke (coal is not present at this point since it enters at the tuyeres in the bottom), while the index of summation i must include SiO_2, Al_2O_3, CaO, MgO and also C (which has not been yet consumed in the thermal reserve zone). As it happened with the sensible heat of slag, l, the amount of coke will be unknown until the Rist diagram is solved, so either an equation solver is used or an iterative process must be followed.

$$C_{\Delta T_R} = Y_W \cdot q_{\mathrm{Fe_{0.95}O}} + (Y_R - Y_W) \cdot \frac{q_{\mathrm{Fe_3O_4}}}{Y_M^*} + \sum_j \sum_i \left(\frac{10^3 \Omega_{\mathrm{j,i}} \mathrm{m_j}}{\mathrm{M_i}\, n_{\mathrm{HM,Fe}}} q_{R,\mathrm{i}} \right) \tag{111}$$

The terms $q_{\mathrm{Fe_{0.95}O}}$, $q_{\mathrm{Fe_3O_4}}$ and $q_{R,\mathrm{i}}$ are the sensible heat of the corresponding element, calculated by Eq.(112) and tabulated in **Table 6** (due to the construction of Eq.(114), we must substitute T by $T_R - \Delta T_R$, and therefore the parameters of $q_{R,i}$ and $q_{l,i}$ have different sign in **Table 6**). The difference with $q_{l,i}$ is that in this case we do not include the heat of fusion. As in the case of l, we neglect the components MnO and P_2O_5 since their contribution in the energy balance is minor.

$$q_{R,i} = \int_{T_R - \Delta T_R}^{T_R} c_{p,i}\, dT \tag{112}$$

It is worth to mention that it seems that Rist had minor errors in the calculation of $C_{\Delta T_R}$ in his original work [10], which lead him to the conclusion that its effect is near to negligible, when its effect is actually one order of magnitude greater than the effect of δ' and δ when $\Delta T_R > 30$ °C.

A.16 List of q as function of T and T_R

The heats denoted by q in Eq.(37) are adjusted either by Eq.(113) or Eq.(114), and they represent a heat of reaction, a heat of fusion, a sensible heat, or a combination of them. They were calculated using data mainly from Aspen Plus database and from NIST. Specific data from other sources is cited when necessary along the appendixes. The parameters a_i of these equations are tabulated in **Table 6**. For the specific case of the heat of decomposition of coal, $q_{\mathrm{CH_{2a}O_{2b}N_{2c}S_{2d}Z_z},d}$, please see Appendix B.

$$q = a_0 + a_1 T + a_2 T^2 + a_3 T^3 + a_4 T^4 + a_5 T^5 \tag{113}$$

$$q = a_0 + a_1 (T - T_R) + a_2 (T^2 - T_R^2) + a_3 (T^3 - T_R^3) + a_4 (T^4 - T_R^4) + a_5 (T^5 - T_R^5) \tag{114}$$

Table 6. Parameters of Eq.(113) and Eq.(114) for the calculation of heats denoted by q (heat of reaction, sensible heat, heat of fusion, or a combination of them). The parameters in this table are already given with the proper sign according to their position in the energy balance of Eq.(37). Data were adjusted in a wide range of temperatures to cover the operating conditions of blast furnace and the typical temperatures of injection in the tuyeres. See units in the nomenclature list.

Term	**Eq.**	a_0	$a_1 \cdot 10^3$	$a_2 \cdot 10^6$	$a_3 \cdot 10^9$	$a_4 \cdot 10^{13}$	$a_5 \cdot 10^{16}$
q_c	(113)	27.6277930	-1.41815549	4.12842928	-2.75130169	8.96569650	-1.11904405
q_v	(114)	0	15.6189049	2.84890885	-0.71432438	0.74256946	0
q_{iw}	(113)	2.59548525	2.81753858	-0.99606163	0.086920157	0	0
q_{im}	(113)	0.859445565	-0.851066970	17.18252955	-24.10333630	126.5591818	-23.40551798
q_{ε}	(113)	10.09226426	-2.622646073	0.207399547	0.018499206	0	0
q_g	(113)	39.94798938	2.612463578	-6.717602910	4.175812336	-13.08493402	1.596921902
q_{er}	(113)	30.09777648	3.812836330	-4.376962349	2.238032117	-6.670590754	0.811140814
q_{es}	(114)	0	-7.811260227	-1.211331943	-0.290874925	1.152621724	0
$q_{js,\mathrm{C}}$	(114)	0	-1.892676053	-4.302515390	2.533624229	-7.781074457	0.945154899
$q_{js,\mathrm{H_2}}$	(114)	0	-7.186451796	0.703157212	-0.990666896	3.831348892	-0.526720187
$q_{js,\mathrm{O_2}}$	(114)	0	-6.918539590	-1.270122896	0.209624517	1.081052901	-0.391217761
$q_{js,\mathrm{N_2}}$	(114)	0	-6.940261215	-0.027976126	-1.017332498	0.062883870	-1.213422894
$q_{js,\mathrm{S_2}}$	(114)	0	-7.765487359	-1.916979150	1.795874077	-8.500453347	1.534226748
$q_{js,\mathrm{Z}}/\mathrm{MW_Z}$	(114)	0	-0.180125344	-0.0699977	0	0	0
q_S	(113)	3.120295853	-1.659566914	4.651898976	-2.732009370	5.882711159	0
$q_{\mathrm{CH4},d}$	(113)	18.75059048	8.630351668	-5.523977040	0.986086895	1.092848019	-0.429883603
$q_{\mathrm{CO2},d}$	(113)	95.20223495	-0.163909537	1.261058571	-0.888254503	2.048695604	-0.018479841
$q_{\mathrm{CO},d}$	(113)	27.63605349	-1.574462606	4.715185141	-3.561402315	13.63334936	-2.073317965
$q_{\mathrm{H2O},d}$	(113)	57.71443993	2.525892875	-0.684828686	0	0	0
q_{Si}	(113)	69.27049820	0.926011273	-9.106679548	6.211945102	-24.51444450	3.691837294
q_{Mn}	(113)	64.39221737	0.899351591	-4.241268160	4.984768433	-25.97307076	5.095307673
q_{P}	(113)	62.25489996	-3.534696289	-1.549594462	0.203580420	0	0
$q_{\gamma\mathrm{Fe}}$	(113)	8.3	0	0	0	0	0
$q_{\mathrm{Fe_3C}}$	(113)	4.739686419	3.895790717	-5.384478435	0.585353566	0	0
$q_{f,\mathrm{Fe}}$	(114)	3.29846	6.272019761	0.999375557	0	0	0
$q_{f,\mathrm{Si}}$	(114)	11.992	5.410629044	0.587816263	0	0	0
$q_{f,\mathrm{Mn}}$	(114)	3.8934	7.486148803	1.310221357	0	0	0
$q_{f,\mathrm{P}}$	(114)	0.1574	6.292069790	0	0	0	0
$q_{f,\gamma\mathrm{Fe}}$	(114)	3.1583	2.581965355	2.386317417	-0.585341267	0	0
$q_{f,\mathrm{Fe_3C}}$	(114)	2.9146	2.581965355	2.386317417	-0.585341267	0	0
$q_{l,\mathrm{SiO_2}}$	(114)	1.83887	15.73272597	0.714132724	0	0	0
$q_{l,\mathrm{Al_2O_3}}$	(114)	25.5565	25.56135703	2.478548686	0	0	0
$q_{l,\mathrm{CaO}}$	(114)	12.4916	11.58470766	0.772858739	0	0	0
$q_{l,\mathrm{MgO}}$	(114)	13.7695	10.89566202	0.762574946	0	0	0
$q_{\mathrm{Fe_{0.95}O}}$	(114)	0	-12.89824855	-1.404696556	-3.264582911	0	0
$q_{\mathrm{Fe_3O_4}}$	(114)	0	-51.12090518	-0.203226315	0.648765211	0	0
$q_{R,\mathrm{SiO_2}}$	(114)	0	-15.73272597	-0.714132724	0	0	0
$q_{R,\mathrm{Al_2O_3}}$	(114)	0	-25.56135703	-2.478548686	0	0	0
$q_{R,\mathrm{CaO}}$	(114)	0	-11.58470766	-0.772858739	0	0	0
$q_{R,\mathrm{MgO}}$	(114)	0	-10.89566202	-0.762574946	0	0	0
$q_{R,\mathrm{C}}$	(114)	0	-1.892676053	-4.302515390	2.533624229	-7.781074457	0.945154899
$q_{s,\mathrm{C}}$	(114)	0	1.892676053	4.302515390	-2.533624229	7.781074457	-0.945154899
$q_{s,\mathrm{N_2}}$	(114)	0	6.889861828	0.375357941	0.421099425	-2.467676481	0.388118345
$q_{s,\mathrm{CO}}$	(114)	0	6.892443	0.351944	0.760803	-5.532971	1.161065
$q_{s,\mathrm{H_2}}$	(114)	0	7.186451796	-0.703157212	0.990666896	-3.831348892	0.526720187
$q_{s,\mathrm{Z}}/\mathrm{MW_Z}$	(114)	0	0.180125344	0.0699977	0	0	0