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1 INTRODUCTION AND DISCLAIMER

This document has been prepared as a user guide to the basic oxygen steelmaking (BOS) simulation, available at http://www.steeluniversity.org/. The interactive simulation has been designed as an educational and training tool for both students of ferrous metallurgy and for steel industry employees.

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2 UNDERLYING SCIENTIFIC RELATIONSHIPS

This section presents the key underlying scientific theories and relationships that are required in order to successfully complete the simulation. In no way is it designed to be comprehensive treatments of steelmaking theory and practice – for this, the user is directed to other excellent publications.

2.1 Calculating Additions

Scrap, slag and iron ore additions are made to the furnace for a variety of reasons

- To adjust the liquid metal temperature
- To adjust the liquid metal composition.
- To change the slag composition and thereby its properties.

2.1.1 Elemental Additions

In the simplest case where a pure element is added, the amount of additive required, \( m_{\text{additive}} \) is simply given by:

\[
m_{\text{additive}} = \frac{\Delta \% X \times m_{\text{steel}}}{100}\]

Where:

\( \Delta \% X \) = required increase in \( \% X \) (i.e. \( \% X_{\text{aim}} - \% X_{\text{current}} \))

\( m_{\text{steel}} \) = mass of steel

Example: Suppose 250,000 kg of steel currently contains 0.01% Ni. How much elemental Ni must be added to achieve an aim composition is 1.0% Ni?
2.1.2 Pickup of Other Elements
When adding scrap it is also important to be aware of, and if necessary calculate, the effect of elements other than iron on the overall steel composition. The new content of a given element is calculated by Equation 9-3:

\[
\%X_{\text{steel,after}} = \frac{m_{\text{scrap}} \times \%X_{\text{scrap}} \times \text{recovery rate of } X + m_{\text{steel}} \times \%X_{\text{steel}}}{100 \times (m_{\text{scrap}} + m_{\text{steel}})}
\]

where

- \(\%X_i\) = content of element in wt-%
- \(m_{\text{slag}}\) = mass of slag in kg
- \(m_{\text{steel}}\) = mass of steel in kg

Example: Calculate the new content of carbon when 10,000 kg of Heavy Scrap is added to 250,000 kg of Hot Metal. Hot Metal contains 4.5\%C (Table 2), Heavy Scrap contains 0.05\%C (Table 2) and carbon has got a 95\% recovery rate (Table 3).

\[
\%C_{\text{steel,after}} = \frac{10,000 \times 0.05 \times 95 + 250,000 \times 4.5}{100 \times (10,000 + 250,000)} = 4.33\%C
\]

Evidently adding large amounts of scrap noticeably reduces the carbon content. However, it is not possible to dilute the hot metal to the required carbon content only by adding scrap. Such a large scrap addition would cause the whole melt to solidify in the furnace.

2.1.3 Mixing Times
Note that that additions made do not result in instantaneous changes to the steel composition, but take a finite time to dissolve. In the simulation, be sure to allow sufficient time for additions to melt and dissolve by observing the following trends:

- Scrap additions dissolve faster than slag or iron ore additions
- Blowing of oxygen accelerates the dissolution process since the oxidation reactions that take place adds heat to the system

You can expect well-stirred additions made at higher temperatures to dissolve faster than additions made at lower temperatures and/or with less stirring.

2.2 Important Reactions
The hot metal charge is refined by rapid oxidation reactions on contact with the injected oxygen with the other elements present under conditions far removed from thermodynamic equilibrium. The three most important reactions are:

\[
[C] + \frac{1}{2}O_2 = CO(g)
\]

\[
[C] + [O] \rightarrow CO(g)
\]

\[
CO(g) + \frac{1}{2}O_2 \rightarrow CO_2(g)
\]
Post-combustion of CO into CO₂ (Equation 9-6) is only partial, i.e. only a part of the present CO will oxidize into CO₂. These gaseous reaction products (CO and CO₂) are evacuated through the exhaust hood. The ratio CO₂/(CO+CO₂) is called Post-Combustion Ratio (PCR).

Other important reactions that the simulation takes into account include:

\[ [\text{Si}] + O₂ = \text{SiO}_2 \]
\[ 2[\text{P}] + \frac{2}{5}O₂ = \text{P}_2\text{O}_5 \]
\[ [\text{Mn}] + \frac{1}{2}O₂ = \text{MnO} \]
\[ [\text{Fe}] + \frac{1}{2}O₂ = \text{FeO} \]
\[ 2[\text{Fe}] + \frac{3}{2}O₂ = \text{Fe}_2\text{O}_3 \]

These oxides combine with previously charged oxides, e.g. lime and dolomite, to form a liquid slag which floats on the surface of the metal bath. The composition of the slag is of utmost importance since it controls many different properties, such as:

- Sulfur partition ratio, \( L_s \)
- Phosphorus partition ratio, \( L_p \)
- Manganese partition ratio, \( L_{Mn} \)
- Liquidus temperature of the slag.

Each of these ratios indicate how the element will be distributed between the slag and the steel, i.e. \( L_p = 1 \) indicates that the level of phosphorus in the steel, [%P], is equal to the level in the slag, (%P).

2.2.1 Phosphorus Partition Ratio

Dephosphorization during the latter part of the basic oxygen steelmaking process is very important because the conditions are favorable compared to other processes within primary and secondary steelmaking. It is therefore critical to maintain a slag composition that improves the phosphorus removal.

Figure 9-1 shows how the phosphorus partition ratio varies with different slag compositions. Maintaining a high ratio is quite difficult since it exists only in a very narrow composition range. Additionally, a temperature increase of 50 °C leads to a decrease of \( L_p \) with a factor of 1.6 at a basicity ratio (CaO/SiO₂) of 3.

\[ L_p = \frac{[\%P]_{\text{slag}}}{[\%P]_{\text{steel}}} \]  
(at equilibrium)

Figure 1: \( L_p \) in the system CaO-SiO₂-FeO-2%P₂O₅-1.5%Al₂O₃-3%MnO-5%MgO at 1650 °C
2.2.2 Dephosphorization Kinetics During Post-Blow Stir

The rate at which the steel is dephosphorized during the post-blow stirring with e.g. nitrogen or argon is controlled by

\[
\frac{d\%P}{dt} = k_c \times \frac{A}{V} \times \left[\%P - \%P_{eq}\right] = -\beta \times \frac{D_p \times Q}{A} \times \frac{A}{V} \times \left[\%P - \%P_{eq}\right]
\]

where

\[k_c = \text{mass transfer coefficient of P in molten steel}\]

\[A = \text{cross sectional area at the slag-metal interface (m}^2\text{)}\]

\[V = \text{steel volume (m}^3\text{)}\]

\[\%P = \text{P content in the steel at time t}\]

\[\%P_{eq} = \text{equilibrium P content at time t}\]

\[b = \text{empirical coefficient (~500 m}^{-1/2}\text{)}\]

\[D_p = \text{P diffusion coefficient in liquid steel (m}^2\text{s}^{-1}\text{)}\]

\[Q = \text{volumetric gas flow-rate across the interface (m}^3\text{s}^{-1}\text{)}\]

2.2.3 Sulfur Partition Ratio

Although desulfurization is not a priority in BOS, there will still be a limited removal of S due to slag/metal interface reactions. Figure 9-2 shows how the sulfur partition ratio varies with slag composition. Please note that in the domain of liquid slags, \(L_s\) is practically temperature independent.

\[L_s = \frac{[\%S]_{slag}}{[\%S]_{steel}} \text{ (at equilibrium)}\]

Figure 2: \(L_s\) in the system CaO-SiO\(_2\)-FeO-2\%P:O\(_2\)-1.5\%Al:O\(_3\)-3\%MnO-5\%MgO at 1650 °C

2.2.4 Manganese Partition Ratio

Most of the manganese present in the hot metal will be oxidized during the first part of oxygen blowing. Any remaining manganese may also be picked up by the slag or reverted back to the steel due to oxidization/reduction reactions at the slag/metal interface.

The manganese partition ratio is slightly temperature dependant. An increased temperature with 50 °C leads to a decrease of \(L_{Mn}\) with a factor of ~1.25.
3 WRITING HEAT AND MASS BALANCES

3.1 Introduction

Mass and heat balances are basic tools for:

- Charge computation
- Adjustment of the composition of certain entities (slag, etc.)
- Adjustment of steel temperature
- Diagnostic to evaluate materials and heat losses

3.2 Mass Balance

In a batch reactor, i.e. where vessel is emptied in between heats, the mass balance compares materials inputs and outputs on the basis of their measured weights and analyses. The difference between the two terms, if any, can be attributed to uncertainties on these parameters, or to a poor identification of some of the inputs (refractory wear, slag carry-over, etc.) or outputs (fumes, dusts, etc.):

$$\sum_{\text{input}} = \sum_{\text{output}} (+\text{losses})$$

One can consider:

- global balances
- balance for certain entities (gas, slag, etc.)
- elementary balances (Fe, O\(_2\), CaO, etc.)

For instance, the balance for element X is written:

$$\frac{1}{100} \sum_{i} Q_{E_i} \cdot \%X_{E_i} = \frac{1}{100} \sum_{j} Q_{S_j} \cdot \%X_{S_j} (+\text{losses})$$

Depending on the context, this equation can be used for:
• Estimating loss terms
• Evaluating the amount $Q_{E_i}$ or $Q_{S_j}$ of an input or output
• Evaluating the composition $%X_{E_i}$ or $%X_{S_j}$ of an input or output

Establishing accurate mass balances is always the crucial first step to guarantee the validity of the energy balance.

3.3 Heat Balance

3.3.1 Thermodynamic Functions and Units:
The thermodynamic function measuring heat exchanges is enthalpy $H$. For a given material, the enthalpy change as a function of temperature, in the absence of phase transformation, is expressed from the heat capacity $C_P$:

$$H_{T_2} - H_{T_1} = \int_{T_1}^{T_2} C_P \cdot dT$$

The SI enthalpy unit is the Joule (J). Other practical units are:

- Calorie (cal): 1 cal = 4.184 J
- Thermie (th): 1 th = 10^6 cal
- Kilowatt-hour (kWh): 1 kWh = 3.6 MJ = 0.86 th

A digest of basic data for Iron & Steelmaking applications, expressed as enthalpy variations of various materials with temperature, phase transformations and chemical reactions is given in the tables below.

3.3.2 Principles for the Establishment of Heat Balance
A practical method for expressing the heat balance consists of collecting the transformations individually for each relevant chemical element, and summing-up at the end. For this calculation, the second principle of the first law of thermodynamics is used: “the heat of reaction depends only on the initial and final states, and not on the intermediate states through which the system may pass”. It is thus sufficient to express the enthalpy of chemical transformations at an arbitrary reference temperature (for instance 1600 °C for a full charge calculation, or the initial steel temperature for a simple temperature adjustment treatment) and to express the enthalpy variations of reactants (respectively reaction products) between their initial (respectively final) states and this reference temperature. For instance, the process sketched below can be used:

$$\Delta H_1 + \Delta H_R + \Delta H_2 + \text{heat loss} = 0$$

![Figure 4: Calculation scheme for a heat balance.](image)
The data in Tables 9.1 to 9.4 are used to compute the terms $\Delta H_1$, $\Delta H_2$, and $\Delta H_R$. The values of $\Delta H_R$ are given for reactants and reaction products at 1600 °C. They are as a first approximation independent of temperature over a domain of several hundred degrees. Note that these terms are positive for endothermic reactions, and negative for exothermic reactions. Depending on the application, this heat balance, coupled with the relevant materials balances, can be used for:

- Charge diagnostic (e.g. evaluation of heat losses)
- Charge calculation (calculation of amounts of materials to be charged to obtain liquid steel at a desired temperature)
- Temperature adjustment calculation (steel temperature variation for addition and reaction of exothermic or endothermic materials). Note that the term $\Delta H_2$ evaluated from equation (4), represents the enthalpy variation of the output materials (liquid steel, slag and possibly gas evolved during the operation) for the temperature difference $\Delta T_{\text{steel}} = T_F - T_i$. The steel temperature change, using $C_p$ values in Table 9.1, is then:

$$
\Delta T_{\text{steel}} = \frac{\Delta H_2}{0.82 Q_{\text{steel}} + 2.04 Q_{\text{slag}}}
$$

where

$\Delta H_2 = \text{sum of heating enthalpies in MJ}$

$Q_{\text{steel}} = \text{mass of steel in tonnes}$

$Q_{\text{slag}} = \text{mass of slag in tonnes}$

### Table 1: Enthalpy values for materials as a function of temperature.

<table>
<thead>
<tr>
<th>Material</th>
<th>$H(1400^\circ\text{C}) - H(25^\circ\text{C})$ / MJ kg$^{-1}$</th>
<th>$C_p$ at 1400 °C / kJ K$^{-1}$ kg$^{-1}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hot metal (liquid at 1400 °C)</td>
<td>1.30 to 1.37</td>
<td>0.87</td>
</tr>
<tr>
<td>Low-alloyed steel (liq at 1600 °C)</td>
<td>1.35</td>
<td>0.82</td>
</tr>
<tr>
<td>Refining slag (liq at 1600 °C)</td>
<td>2.14</td>
<td>2.04</td>
</tr>
<tr>
<td>Iron ore Fe$_3$O$<em>4$ (= Fe$</em>{10}$ + O)</td>
<td>4.43</td>
<td></td>
</tr>
<tr>
<td>CaO</td>
<td>1.50</td>
<td>1.03</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Material</th>
<th>$H(1600^\circ\text{C}) - H(25^\circ\text{C})$ / MJ kg$^{-1}$</th>
<th>$C_p$ at 1600 °C / kJ K$^{-1}$ kg$^{-1}$ / kJ K$^{-1}$ m$^{-3}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ar</td>
<td>0.82</td>
<td>1.46 / 0.53 / 0.93</td>
</tr>
<tr>
<td>CO</td>
<td>1.86</td>
<td>2.33 / 1.28 / 1.61</td>
</tr>
<tr>
<td>CO$_2$</td>
<td>1.90</td>
<td>3.78 / 1.36 / 2.71</td>
</tr>
<tr>
<td>N$_2$</td>
<td>1.84</td>
<td>2.30 / 1.28 / 0.95</td>
</tr>
<tr>
<td>O$_2$</td>
<td>1.70</td>
<td>2.43 / 1.17 / 1.68</td>
</tr>
</tbody>
</table>
Table 2: Enthalpy of oxidation reactions for various elements.

<table>
<thead>
<tr>
<th>Element X to Oxide $X_{2}O_{m}$</th>
<th>Heating from 25 to 1600 °C + dissociation / MJ kg$^{-1}$</th>
<th>$C_e$ element X at 1600 °C / kJ K$^{-1}$ kg$^{-1}$</th>
<th>Oxidation X at 1600 °C by dissolved $O_2$ / MJ kg$^{-1}$</th>
<th>Oxidation X at 1600 °C by $O_2$ gas at 25 °C / MJ kg$^{-1}$</th>
<th>Amount $O_2$ / kg</th>
<th>/ m$^3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>C in CO</td>
<td>4.26 to 6.0$^{(*)}$</td>
<td>2.925</td>
<td>-1.03 to -3.37$^{(*)}$</td>
<td>-9.4 to -10.84$^{(*)}$</td>
<td>1.33</td>
<td>0.93</td>
</tr>
<tr>
<td>C in CO$_2$</td>
<td>4.26 to 6.0$^{(*)}$</td>
<td>2.925</td>
<td>-15.35 to -16.79$^{(*)}$</td>
<td>-30.35 to -31.79$^{(*)}$</td>
<td>2.67</td>
<td>1.87</td>
</tr>
<tr>
<td>Al in Al$_2$O$_3$</td>
<td>-0.17</td>
<td>1.175</td>
<td>-22.32</td>
<td>-27.32</td>
<td>0.89</td>
<td>0.62</td>
</tr>
<tr>
<td>Cr in Cr$_2$O$_3$</td>
<td>1.37</td>
<td>0.95</td>
<td>-7.76</td>
<td>-10.36</td>
<td>0.46</td>
<td>0.32</td>
</tr>
<tr>
<td>Fe in &quot;FeO&quot; liq</td>
<td>1.35</td>
<td>0.82</td>
<td>-2.49</td>
<td>-4.10</td>
<td>0.29</td>
<td>0.20</td>
</tr>
<tr>
<td>Fe in Fe$_2$O$_3$</td>
<td>1.35</td>
<td>0.82</td>
<td>-4.06</td>
<td>-6.48</td>
<td>0.43</td>
<td>0.30</td>
</tr>
<tr>
<td>Mn in MnO</td>
<td>1.53</td>
<td>0.835</td>
<td>-5.34</td>
<td>-6.07</td>
<td>0.29</td>
<td>0.20</td>
</tr>
<tr>
<td>P in Cr$_2$P$^{(*)}$</td>
<td>-0.14</td>
<td>0.61</td>
<td>-23.8</td>
<td>-31.05</td>
<td>1.29</td>
<td>0.90</td>
</tr>
<tr>
<td>Si in Cr$_2$S$^{(***)}$</td>
<td>-1.43</td>
<td>1.43</td>
<td>-24.4</td>
<td>-29.35</td>
<td>1.14</td>
<td>0.80</td>
</tr>
</tbody>
</table>

$^{(*)}$ in liquid steel  
$^{(***)}$ in hot metal  
$^{(****)}$ to form 3 CaO-P$_2$O$_5$ and 2 CaO-SiO$_2$ with necessary CaO taken at 1600 °C

Table 3: Reactions of oxygen dissolution in liquid steel at 1600 °C (MJ/kg O$_2$).

<table>
<thead>
<tr>
<th>From O$_2$ gas at 25 °C</th>
<th>From FeO$_2$ in slag at 1600 °C</th>
<th>From very stable oxides at 1600 °C</th>
</tr>
</thead>
<tbody>
<tr>
<td>- 5.62</td>
<td>8.7</td>
<td>18</td>
</tr>
</tbody>
</table>

Table 4: Enthalpy of decomposition of ferroalloys at 25°C (MJ/kg alloy).

<table>
<thead>
<tr>
<th>High C Ferro-Cr (64%Cr 5%Cr)</th>
<th>Refined Ferro-Cr (73%Cr 0.5%C)</th>
<th>High C Ferro-Mn (78%Mn 7%Cr)</th>
<th>Refined Ferro-Mn (80%Mn 1.5%Mn)</th>
<th>Ferro-Silicon (75%Si)</th>
<th>Ferro-Silicon (50%Si)</th>
<th>Silico-Manganese (35%Si)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.11</td>
<td>- 0.025</td>
<td>0.10</td>
<td>0.075</td>
<td>0.37</td>
<td>0.70</td>
<td>0.71</td>
</tr>
</tbody>
</table>

3.3.3 Example of Application: Steel Heating by Aluminothermy

Take the calculation of the change in steel temperature as an example of a heat and mass balance. Initially at 1620 °C, what will the steel temperature be after the addition of 1 kg Al (+O$_2$ gas) per tonne of steel?

Applying the heat balance shown in Equation 10-4 provides the necessary parameters.

The materials balance indicates that 0.89 kg O$_2$ are necessary per kg Al, and that 1.89 kg Al: O$_3$ are formed (see Table 10-2).

1) Calculation of $\Delta H_1$: - 5.13 MJ including:
   a) Heating and dissolution of 1 kg Al:
      i) $-0.17$ MJ (heating at 1600 °C + dissolution, see Table 10-2)
      ii) $+1.175 \times 10^{-3} \times 20$ (heating from 1600 to 1620 °C)
   b) Heating and dissolution of 0.89 kg O$_2$:
   c) $-5.62 \times 0.89$ MJ (heating at 1600 °C + dissolution, see Table 10-3)
   d) $+1.17 \times 10^{-3} \times 20 \times 0.89$ (heating from 1600 to 1620 °C)

2) Calculation of $\Delta H_R$: -22.32 MJ (see Table 10-2)

3) Thus, $\Delta H_2 = -(\Delta H_1 + \Delta H_R) = 27.45$ MJ
The corresponding temperature change for 1 tonne of steel, taking into account a typical slag weight of 20 kg/tonne (including formed $\text{Al}_2\text{O}_3$) and neglecting heat losses is:

$$\Delta T_{\text{steel}} = \frac{27.45}{0.82 + 2.04 \times 0.020} = 31.9^\circ\text{C}$$

If the reaction takes place using dissolved oxygen instead of gaseous oxygen, it is necessary to subtract from $\Delta H_1$ the enthalpy of dissolution of oxygen, i.e. (-5.62 x 0.89 MJ/kg Al). The temperature change is then:

$$\Delta T_{\text{steel}} = \frac{27.45 - 5.62 \times 0.89}{0.82 + 2.04 \times 0.020} = 26.1^\circ\text{C}$$

If the reaction takes place using oxygen resulting from the reduction of iron oxides in the slag, it is necessary to add to this last value of $\Delta H_1$ the enthalpy of decomposition of FeO$x$, i.e. (8.7 x 0.89 MJ/kg Al). In this case, the temperature change would be:

$$\Delta T_{\text{steel}} = \frac{27.45 - 5.62 \times 0.89 - 8.7 \times 0.89}{0.82 + 2.04 \times 0.020} = 17.1^\circ\text{C}$$

4 CHARGE CALCULATION

4.1 Choice of Balance Equations

The reaction products between hot metal and oxygen enter either the slag (Fe, Si, Mn, P, Cr etc.) or the gas (C as CO and CO2) phase. The distribution of elements between liquid metal, slag and gas depends on the amount of blown oxygen and on the conditions of contact between hot metal and oxygen. The blowing conditions will influence:

- Gas composition; post-combustion ratio $\text{PCR} = \text{CO}_2 \div (\text{CO} + \text{CO}_2)$ where CO and CO2 are volumetric fractions.
- Oxidation degree of Fe in the slag $\text{Fe}^{3+} / (\text{Fe}^{2+} + \text{Fe}^{3+})$. In top blowing, this ratio is about 0.3 which corresponds to a mass ratio $\text{O}_{\text{linked}} / \text{Fe}_{\text{oxidized}} = 0.33$.

In addition, it is necessary to impose a constraint on the amount of oxidized Fe, usually through a fixed value of the slag iron content. For stainless steels, oxidation of Cr is considered, usually fixed through the oxygen decarburization yield.

In this simplified system, it is clear that for a steel of given composition, and once the three discussed parameters are fixed (gas composition, oxidation degree and amount of oxidize Fe), 4 equations are necessary in order to evaluate the amounts of oxygen, liquid steel, slag and gas corresponding to the treatment of a given amount of hot metal (or to produce a given amount of steel). These equations are the balances of Fe, O, gas, and slag elements other than Fe (Si, Mn and P). It can easily be shown that these equations are independent.

Any additional constraint will require an additional input variable (or the release of one of the previous constraints). This is the case for typical industrial conditions:

- The steel temperature is fixed. This constraint requires charging an endothermic (scrap, ore, etc.) or exothermic (ferrosilicon, coal, etc.) agent.
- Burnt lime addition for desired slag properties. This constraint can be expressed as an additional imposition on slag composition (CaO content, or basicity-ratio CaO/SiO$_2$ or (CaO+MgO)/(SiO$_2$+P$_2$O$_5$), or imposition of a burnt lime rate equation.
Fixation of the slag MgO content for lining protection. An independent MgO input is necessary, for instance as dolomitic lime.

Table 5: Input and Output material from the Basic Oxygen Steelmaking Process.

<table>
<thead>
<tr>
<th>Input</th>
<th>Output</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Liquid steel</td>
</tr>
<tr>
<td>Hot metal</td>
<td>Weight fixed (or unknown) ( P_{Fe} ), composition and temperature fixed</td>
</tr>
<tr>
<td>Scrap or Ore</td>
<td>Weight unknown ( P_{Fe} ) or ( P_{Si} ), composition and temperature fixed</td>
</tr>
<tr>
<td>Burnt lime</td>
<td>Weight unknown ( P_{Casa} ), composition and temperature fixed</td>
</tr>
<tr>
<td>Oxygen</td>
<td>Weight unknown ( P_{O} ), composition and temperature fixed</td>
</tr>
<tr>
<td>Slag</td>
<td>Weight unknown ( P_{L} ), temperature fixed</td>
</tr>
<tr>
<td></td>
<td>Iron oxide and oxidation degree fixed ( \Rightarrow %Fe_{x}, %O_{y} )</td>
</tr>
<tr>
<td></td>
<td>Complete composition will be computed from elementary balances (Si, P, etc.)</td>
</tr>
<tr>
<td>Gas</td>
<td>Weight unknown ( P_{O} )</td>
</tr>
<tr>
<td></td>
<td>Average temperature and post-combustion ratio ( PCR ) fixed</td>
</tr>
</tbody>
</table>

Thus, a typical charge with the minimum amount of required materials has 6 unknowns and requires 6 balance equations:

- Fe balance
- O balance
- Gas balance
- Balance of slag elements other than Fe
- Basicity equation balance
- Energy balance

4.2 Principle of Using the Simplex Method to Solve the Balance Equations

In general, more materials than strictly necessary are available to make-up the charge (various scrap qualities, ferroalloys, etc.). A practical way to compute the optimal charge (minimal cost for a given steel grade) is to use the Simplex Algorithm which is a minimization of the objective function charge cost \( z = f(c,P) \), a linear equation in terms of weights of the various materials:

\[
z = \sum_{j} c_{j} \cdot P_{j}
\]

Where

- \( P_{j} \) = weights of the various concerned materials (hot metal, scraps, etc., slag, gas)
- \( c_{j} \) = cost including costs linked to their use, and possibly disposal costs (slag) or valorization (gas)

The variables \( P_{j} \) are submitted to the balances constraints, as well as other possible constraints of materials availability, analytical limits, etc.:

\[
\sum_{j=1}^{n} a_{ij} \cdot P_{j} \begin{cases} \leq, =, \geq \end{cases} b_{j} \quad i = 1,...,m
\]
Among the materials availability constraints, we may impose maximum or minimum weights of certain materials (e.g. provision of a minimal amount of ore for final temperature adjustment), or of certain materials assemblies (e.g. maximal capacity in weight and volume of the scrap boxes), impose the weight of certain materials (e.g. solid iron, internal scrap).

Among analytical limits constraints, we may impose a maximal steel Cu (or other tramp elements) content, the slag MgO content for lining protection, etc.

The possibility, with the Simplex Method, to impose arbitrarily the weight of certain materials, offers the advantage of using the same calculation module for charge calculation (the weight of liquid steel is fixed and that of hot metal and other charge materials are unknown), and for heat diagnostic calculations (the charged materials are known and the theoretical steel weight is computed, along with actual materials and heat losses).

4.3 11.3 How to Write the Balance Equations

The equations are written here for the standard charge with minimal number of materials. The transposition to a higher number of available materials is direct.

4.3.1 Fe Balance

\[ \left( \% \text{Fe}_{\text{Fe}} \cdot P_{\text{Fe}} + \% \text{Fe}_{\text{Fe}} \cdot P_{\text{Fe}} + \% \text{Fe}_{\text{M}} \cdot P_{\text{M}} \right) = \left[ \% \text{Fe}_{\Lambda} \cdot P_{\Lambda} + \% \text{Fe}_{\Lambda} \cdot P_{\Lambda} \right] \]

4.3.2 O Balance

The amounts of oxygen used for the oxidation of the various elements C, Mn, P, Si are computed on the basis of the amounts of these elements oxidized, \( Q_C \), \( Q_{Mn} \), \( Q_p \) and \( Q_{Si} \).

\[ Q_C = 0.01 \left( \% \text{C}_{\text{Fe}} \cdot P_{\text{Fe}} + \% \text{C}_{\text{Fe}} \cdot P_{\text{Fe}} - \% \text{C}_{\Lambda} \cdot P_{\Lambda} \right) \]

(and similarly for Mn, P and Si)

Taking into account the amount of oxygen used for oxidizing Fe computed from the slag composition, and the amount of dissolved oxygen in the steel, the oxygen balance is:

\[ P_{O_3} + 0.01 \cdot \% O_M \cdot P_M = \left[ \frac{16}{12} \cdot (1 - P_{CR}) + \frac{32}{12} \cdot P_{CR} \right] \cdot Q_C + \frac{16}{55} \cdot Q_{Mn} + \frac{80}{62} \cdot Q_p + \frac{32}{28} \cdot Q_{Si} + 0.01 \cdot (\% O_{Fe})_M \cdot P_{\Lambda} + 0.01 \cdot \% O_{\Lambda} \cdot P_{\Lambda} \]

4.3.3 Gas Balance

\[ P_G = \left[ \frac{28}{12} \cdot (1 - T_{CS}) + \frac{44}{12} \cdot T_{CS} \right] \cdot Q_C \]

When using a stirring gas (Ar, N\(_2\), etc.), it is necessary to add \( P_{Ar} \), \( P_{N2} \), etc.

4.3.4 Balance of Slag Elements Other than Fe

\[ \frac{71}{55} \cdot Q_{Mn} + \frac{142}{62} \cdot Q_p + \frac{60}{28} \cdot Q_{Si} + 0.01 \cdot \% \text{CaO}_{Chx} \cdot P_{Chx} \]

\[ = 0.01 \cdot \left[ 100 - \% \text{Fe}_{\Lambda} - (\% O_{Fe}) \right] \cdot P_{\Lambda} \]

4.3.5 Basicity Equation

If, for instance, the basicity ratio \( V = \% \text{CaO}/\% \text{SiO}_2 \) is imposed:
4.3.6 Energy Balance

We use Equation 10-4 of section 10.3 Heat Balance, taking 1600 °C for reference so that the data of Tables 10-1 to 10.4 can be used simply. Note that in these tables, weights are in kg and enthalpy terms in MJ or kJ:

**Step 1**

The charged materials are brought from their initial state to that of elements dissolved in liquid metal at 1600 °C (except burnt lime which is simply heated)

\[ \Delta H_1 = 0.00087 (1600 - T_{Fe})P_{Fe} + \]
\[ +1.35P_{Fe} + 4.43P_{M^+} + \]
\[ +1.5P_{chx} + \]
\[ -5.62P_{o} \]

(heating hot metal - see Table 10-1)

(heating and dissolving scrap and ore - see Table 10-1)

(heating burnt lime - see Table 10-1)

(heating and dissolving oxygen - see Table 10-3)

Also use data from Table 10-4 and the first column of Table 10-2 if ferroalloys are being charged.

**Step 2**

Enthalpy of reactions between dissolved elements at 1600 °C (Table 10-2).

\[ \Delta H_2 = [-3.37 \cdot (1 - PCR) - 16.79 \cdot PCR] \cdot Q_{C} \]
\[ -5.34 \cdot Q_{Mn} - 23.8 \cdot Q_{P} - 24.4 \cdot Q_{Si} - 0.0296 \cdot %Fe_{L} \cdot P_{L} \]

**Step 3**

Steel, slag and gas are brought to their final temperature.

\[ \Delta H_3 = 0.00082(T_{A} - 1600)P_{A^+} + \]
\[ +0.00204(T_{L} - 1600)P_{L^+} + \]
\[ +[0.00128(T_{o} - 1600)](1 - PCR) + [0.00136(T_{o} - 1600)]PCR]Q_{C} \]

(\(\Delta T_{steel}\) - see Table 10-1)

(\(\Delta T_{slag}\) - see Table 10.1)

(\(\Delta T_{gas}\) for CO + CO\(_2\) - see Table 10.1)

Add the following respective term(s) if argon and/or nitrogen stirring gas are used:

**Table 6: Starting values for the heat and mass balance.**

<table>
<thead>
<tr>
<th>Hot metal composition</th>
<th>4.5 %C, 0.5 %Mn, 0.08 %P, 0.4 %Si (that is 94.52 %Fe) at 1350 °C.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Scrap composition</td>
<td>100 %Fe. - No ore.</td>
</tr>
<tr>
<td>Burnt lime</td>
<td>100 %CaO.</td>
</tr>
<tr>
<td>Liquid steel composition</td>
<td>0.05 %C, 0.12 %Mn, 0.01 %P (that is 99.73 %Fe) at 1650 °C.</td>
</tr>
<tr>
<td>Slag</td>
<td>%CaO/%SiO(_2)=4, oxidized Fe content 18% at 1650 °C.</td>
</tr>
<tr>
<td>Gas</td>
<td>PCR=0.08 extracted at an average temperature of 1500 °C.</td>
</tr>
<tr>
<td>Heat losses</td>
<td>65 MJ/t steel.</td>
</tr>
</tbody>
</table>
4.4 Numerical Application

The first step in making a charge calculation for 1 tonne steel is to calculate the amounts of oxidized C, Mn, P and Si:

\[
Q_C = 0.045 \cdot P_{\text{Fe}}^{0.5} \\
Q_{\text{Mn}} = 0.005 \cdot P_{\text{Fe}}^{1.2} \\
Q_P = 0.0008 \cdot P_{\text{Fe}}^{0.1} \\
Q_Si = 0.004 \cdot P_{\text{Fe}}
\]

Then, all 6 heat and mass balance equations are calculated according to Table 11-3:

Table 7: Heat and Mass balance end equations.

<table>
<thead>
<tr>
<th>Equation Type</th>
<th>Equation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fe balance</td>
<td>0.9452 \cdot P_{\text{Fe}} + P_{\text{Fe}} - 0.18 \cdot P_{\text{L}} = 997.30</td>
</tr>
<tr>
<td>O balance</td>
<td>0.0718 \cdot P_{\text{Fe}} + P_{\text{O}} + 0.0544 \cdot P_{\text{L}} = 1.098</td>
</tr>
<tr>
<td>Gas balance</td>
<td>0.1098 \cdot P_{\text{Fe}} - P_{\text{G}} = 1.22</td>
</tr>
<tr>
<td>Balance of slag elements other than Fe</td>
<td>0.0169 \cdot P_{\text{Fe}} + P_{\text{Chx}} - 0.7606 \cdot P_{\text{L}} = 1.778</td>
</tr>
<tr>
<td>Slag basicity</td>
<td>0.0343 \cdot P_{\text{Fe}} - P_{\text{Chx}} = 0</td>
</tr>
<tr>
<td>Energy balance</td>
<td>-0.1287 \cdot P_{\text{Fe}} + 1.35 \cdot P_{\text{Fe}} + 1.5 \cdot P_{\text{Chx}} - 5.62 \cdot P_{\text{O}} - 0.3462 \cdot P_{\text{L}} = -117.2</td>
</tr>
</tbody>
</table>

Finally, the masses are calculated:

\[
P_{\text{Fe}} = 885.3 \text{ kg} \\
P_{\text{Fe}} = 171.6 \text{ kg} \\
P_{\text{Chx}} = 30.4 \text{ kg} \\
P_{\text{O}} = 65.6 \text{ kg} \\
P_{\text{A}} = 1000 \text{ kg} \\
P_{\text{L}} = 57.2 \text{ kg} \\
P_{\text{G}} = 96.0 \text{ kg}
\]

5 BIBLIOGRAPHY
