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Basic Oxygen Steelmaking Simulation, version 1 User Guide

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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 Introduction to Basic Oxygen Steelmaking

Basic oxygen steelmaking (BOS) is the most widely used process for producing crude steel from molten pig iron (hot metal). The process involves blowing oxygen through hot metal to reduce its carbon content by oxidation. There exist many different types of furnaces, also called converters since they are used to convert hot metal to steel, and these are generally divided into top-blowing, bottom-blowing and mixed blowing.

Top-blowing through a vertical lance was invented in 1952-53 at Linz and Donawitz in Austria and the process is known as LD (Linz Donawitz), or BOP (Basic Oxygen Process). Bottom-blowing processes use, apart from oxygen, hydrocarbon gas (propane or natural gas) or fuel-oil hydrocarbon that cools the refractory in the tuyere zone. These corresponding processes are known as OBM (Oxygen Bottom-blowing Maxhütte), Q-BOP (Quick Basic Oxygen Process) and LWS (Loire-Wendel-Sidelor). One of their advantages is a very efficient metal-slag stirring throughout the oxygen blow.

Mixed blowing developed in the late 1970s is the latest step. A limited blowing of neutral gas (argon or nitrogen) or oxygen through the vessel bottom of top-blown converters provides an efficient stirring. The corresponding processes are known as LBE (Lance Bubbling Equilibrium), LET (Lance Equilibrium Tuyeres), K-BOP (Kawasaki Basic Oxygen Process), K-OBM (Kawasaki Oxygen Bottom-blowing Maxhütte) etc. and these facilities now equips most of the top-blown converters.

Hot metal desulfurization is generally carried out prior to the hot metal being charged into the furnace. Different fluxes are used for different levels of sulfur; for example lime, calcium carbide and magnesium.

Hot metal dephosphorization was developed in Japan in the early 1980s. In this pretreatment operation, most of the hot metal P is removed using oxidizing fluxes (mixtures of lime and

iron ore) in the hot metal ladle prior to charging in the converter. This treatment has so far not been applied at all outside of Japan.

3 Simulation Objectives

The aim of the simulation is to take charge of a Basic Oxygen Furnace (BOF), treat the hot metal by making necessary additions and blowing of oxygen, and tap the heat into the ladle at the **specified time, composition and temperature**.

You should also aim to **minimize the cost** of the whole operation.

4 Plant Layout and Description

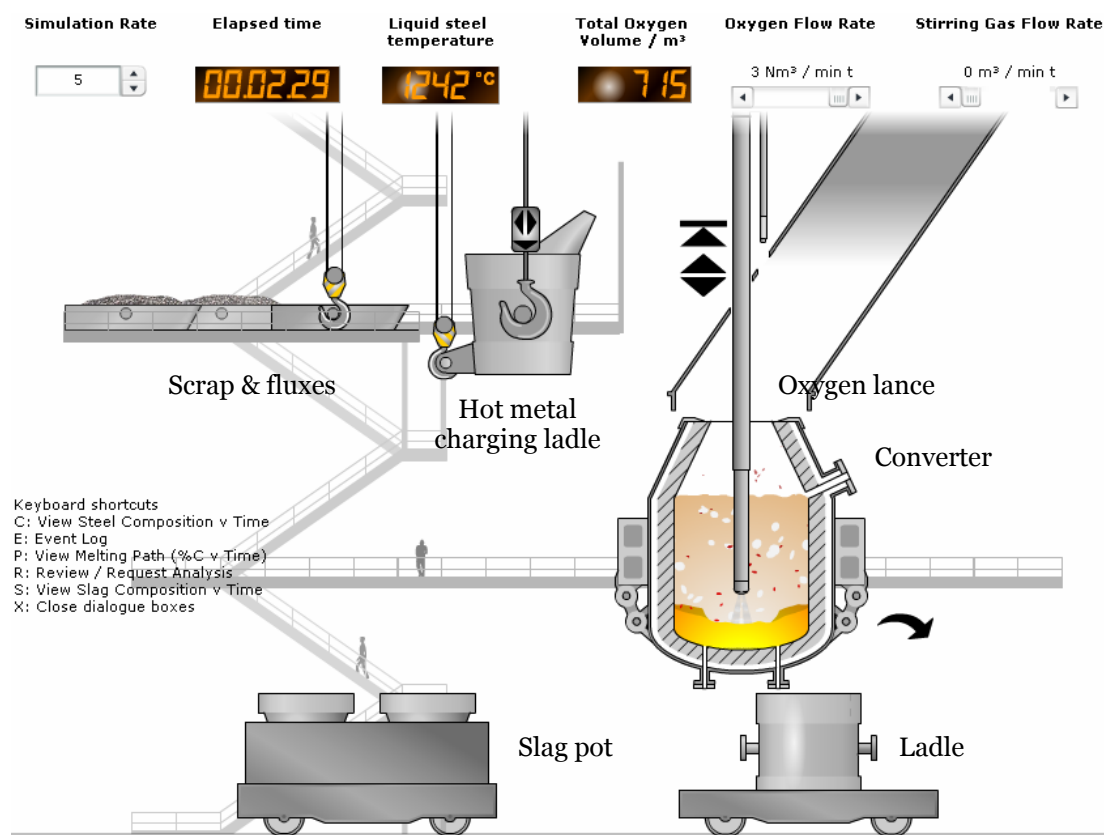


Figure 4-1: Screenshot showing the plant layout used in the simulation.

The plant in the simulation is laid out as shown in Figure 4-1. At the start of the simulation, an animation shows how scrap metal and additives like lime and dolomite (according to the user's choices) are first charged into the furnace. After the solid material has been charged the hot metal is tapped from the transport ladle into the furnace. The simulation ends with a summary screen when the steel has been tapped into the ladle.

5 Simulation Options

5.1 User Levels

The simulation has been developed for use by two different user groups:

- University students of metallurgy, materials science and other engineering disciplines

- Steel industry works technical

5.1.1 UNIVERSITY STUDENT LEVEL

At this level the user will be expected to approach the problem scientifically, using the relevant thermodynamic and kinetic theories to make decisions on the various processing options. For example, the user should perform a full heat and mass balance calculation to determine the amount of scrap and slag additions and the necessary total oxygen volume.

At this level the unmelted solids, e.g. scrap and iron ore, will be visible to the user.

5.1.2 STEEL INDUSTRY WORKS TECHNICAL LEVEL

At this level the user will also be expected to approach the problem scientifically. However, the user will have to complete the simulation with a limited number of aids. For example, the unmelted solids will not be visible at this level.

5.2 Simulation Speed

The simulation can be run at a range of different speeds between $\times 1$ and $\times 32$. The rate can be changed at any time during the simulation. However, when important events take place the simulation will automatically default to $\times 1$.

5.3 Target Steel Grade

The simulation includes a number of different steel grades to illustrate a range of different processing options.

The general-purpose **construction steel grade (CON)** is a relatively undemanding grade that requires minimal processing, and is therefore recommended for the **novice user**. Your main job is to ensure that the carbon content is between 0.1 and 0.16%.

The **TiNb ultra-low carbon steel (ULC)**, for automotive body parts, has a carbon specification of less than 0.01%C with the aims to optimize formability. Your main priority therefore is temperature control at the end of the blow to keep the temperature below maximum whilst achieving the low target content.

The **linepipe steel (LPS)** for gas distribution is a **very demanding** grade as the combination of high strength and high fracture toughness demands extremely low levels of impurities (S, P, H, O and N) and inclusions. Only more experienced users are recommended to attempt this grade.

The **engineering steel (ENG)** is a heat-treatable low alloy grade with a relatively high carbon content. Choosing the correct starting temperature is imperative to achieve the target temperature whilst maintaining the carbon content between 0.30 and 0.45%C.

Table 5-1: Maximum contents for the four target steel grades available in the simulation / wt-%.

Element	CON	ULC	LPS	ENG
C	0.16	0.01	0.08	0.45
Si	0.25	0.25	0.23	0.40
Mn	1.5	0.85	1.1	0.90
P	0.025	0.075	0.008	0.035
S	0.10	0.05	0.01	0.08
Cr	0.10	0.05	0.06	1.2
B	0.0005	0.005	0.005	0.005
Cu	0.15	0.08	0.06	0.35
Ni	0.15	0.08	0.05	0.30
Nb	0.05	0.03	0.018	0
Ti	0.01	0.035	0.01	0
V	0.01	0	0.01	0.01
Mo	0.04	0.01	0.01	0.30
Ca	0	0	0.005	0

Table 5-2: Aim tapping temperatures for the four target steel grades / °C.

	Minimum	Maximum
CON	1630	1660
ULC	1665	1695
LPS	1655	1685
ENG	1655	1685

6 Planning your Schedule

Before you start the simulation, it is important that you plan ahead. The first thing to do is to complete a heat and mass balance calculation to determine the amounts of hot metal, scrap, iron ore, slag additions and total oxygen volume required to decarburize the hot metal to the desired carbon content and temperature. You then need to think how to achieve the aim values within the required time.

Table 6-1: Example Hot Metal and Tapping (Aim) Compositions for the Ultra-Low Carbon steel grade. Carbon, silicon and phosphorus compositions must all be decreased, whereas manganese can be left as is. Also, the temperature will have to be increased.

	Hot Metal / wt%	Tapping / wt%	Difference / wt%
C	4.5	0.01	-4.49
Si	0.4	0.25	-0.15
Mn	0.5	0.85	+0.35
P	0.08	0.075	-0.005
Temperature	1350°C	1680°C	+330°C

6.1 Composition

Some additions will have to be made in order to meet the aim composition. Here are the key questions you will need to answer

- Which additive(s) can be used to achieve this?
- How much additive (in kg) will be required?
- Will this additive affect other elements too and if so, how much?
- When should you make the addition?
- How will the additions affect cost, steel composition and temperature?

Table 6-2: Compositions and costs of available additives.

Additive	Composition	Cost per tonne
Hot Metal	4.5%C, 0.5%Mn, 0.4%Si, 0.08%P, 0.02%S + Fe bal.	\$185
Light scrap	0.05%C, 0.12%Mn, 0.015%P, 0.015%S, 0.06%O, 0.003%Ce, 0.26%Cr, 0.02%Cu, 0.14%Mo, 0.001%Nb, 0.4%Ni, 0.001%Sn, 0.015%Ti, 0.005%V, 0.009%W + Fe bal.	\$190
Heavy scrap	0.05%C, 0.12%Mn, 0.015%P, 0.015%S, 0.06%O, 0.003%Ce, 0.26%Cr, 0.02%Cu, 0.14%Mo, 0.001%Nb, 0.4%Ni, 0.001%Sn, 0.015%Ti, 0.005%V, 0.009%W + Fe bal.	\$150
Iron Ore	99.1%FeO, 0.3%Al ₂ O ₃ , 0.5%CaO, 0.1%MgO, 0.001%P	\$85
Lime	94.9%CaO, 1.2%Al ₂ O ₃ , 1.8%MgO, 2.1%SiO ₂	\$85
Dolomite	59.5%CaO, 38.5%MgO, 2%SiO ₂	\$85

Table 6-3: Typical recovery rates for elements added (%).

Element	C	Si	Mn	P	S	Cr	Al	B	Ni
Recovery rates	95	98	95	98	80	99	90	100	100
Element	Nb	Ti	V	Mo	Ca	N	H	O	Ar
Recovery rates	100	90	100	100	15	40	100	100	100
Element	As	Ce	Co	Cu	Mg	Pb	Sn	W	Zn
Recovery rates	100	100	100	100	100	100	100	100	100

6.2 Temperature

In order that the correct tapping temperature is achieved, it is important to consider the effects of different additions on the steel temperature.

1. Under holding conditions, such as when stirring gas has been turned off and there is no oxygen injection, the steel cools at around 1 to 2°C min⁻¹.
2. For most additions, each tonne (1000 kg) added results in an additional temperature drop of about 5°C.
3. Phosphorus and silicon oxidation is highly exothermic and produces about 26 MJ/tonne per 0.1% per tonne of hot metal oxidized, the equivalent of nearly 3 °C/tonne per 0.1%.
4. Carbon oxidation is also exothermic and produces about 13 MJ/tonne per 0.1% oxidized, the equivalent of about 1.4 °C/tonne per 0.1%.
5. Increasing the hot metal or steel temperature requires 9.0 or 9.4 MJ/tonne, respectively.

By carefully calculating the overall time from charging to tapping the BOF it should be possible to estimate the temperature vs. time profile.

6.2.1 CALCULATION OF LIQUIDUS TEMPERATURE

It is imperative to prevent the steel bath temperature falling below the liquidus temperature (i.e. the temperature at which the steel starts to solidify). The liquidus temperature, T_{liq} , is very dependent on composition and can be approximated from the following equations:

For %C < 0.5:

$$T_{liq} (^{\circ}\text{C}) = 1537 - 73.1\%C - 4\%Mn - 14\%Si - 45\%S - 30\%P - 1.5\%Cr - 2.5\%Al - 3.5\%Ni - 4\%V - 5\%Mo \quad 6-1$$

For 0.5 < %C < 4.4:

$$T_{liq} (^{\circ}\text{C}) = 1531 - 61.5\%C - 4\%Mn - 14\%Si - 45\%S - 30\%P - 1.5\%Cr - 2.5\%Al - 3.5\%Ni - 4\%V - 5\%Mo \quad 6-2$$

For %C > 4.4:

$$T_{liq} (^{\circ}\text{C}) = 389 \%C - 10.5 \%Mn + 105 \%Si + 140 \%S + 128 \%P - 506$$

6.3 Stages of the Oxygen Blowing Process

There are three typical reaction periods during BOP to consider; silicon oxidation, full decarburization and carbon diffusion. These all have distinctly different reaction patterns. An overview can be seen in Figure 6-1.

6.3.1 SILICON OXIDATION PERIOD

During the first third (approximately) of the blow most of the Si is oxidized along with some Fe. A good practice is to increase the FeO content and get a good foaming slag at the very beginning of the blow and then stabilize it by lowering the lance until the foam stops rising.

It is also during this period that most of the P and Mn are oxidized. The remainder of the supplied oxygen reacts with carbon

6.3.2 FULL DECARBURIZATION PERIOD

Under normal conditions, all of the supplied oxygen reacts with carbon. However, if the lance position is too high, a portion of the oxygen will instead oxidize Fe. On the other hand, when the lance is too low, the previously formed FeO (and foaming slag) is reduced and the oxygen released reacts with C.

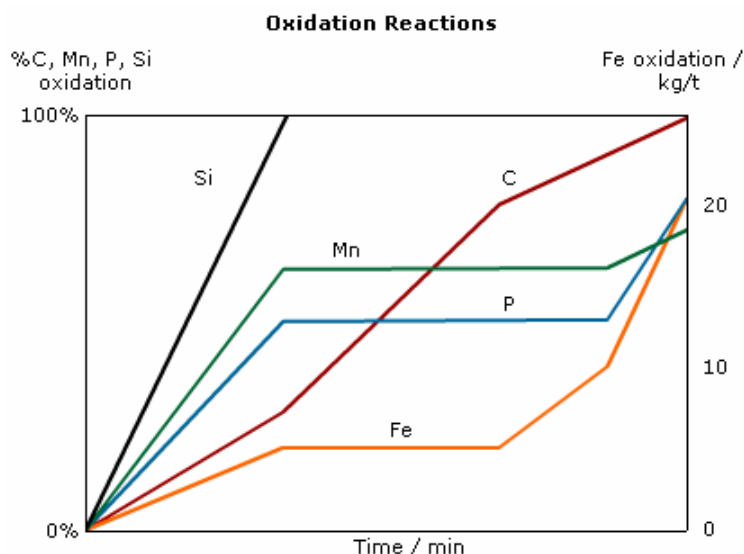


Figure 6-1: Reaction rates for oxidation reactions in BOS.

6.3.3 CARBON DIFFUSION PERIOD

At the end of the blow when the carbon content is less than 0.8%C, the rate of decarburization decreases substantially and is now increasingly limited by the diffusion of carbon in the steel. An approximate equation for decarburization during period is shown in (remaining oxygen will oxidize Fe):

$$\Delta\%C = \frac{V_{O_2}}{0.98 + \frac{0.15}{(\%C)^2}} \quad 6-3$$

where

- $\Delta\%C$ = change in carbon content in wt-%
- $\%C$ = current carbon content in wt-%
- V_{O_2} = oxygen supplied in m³/tonne

7 User Interface

This section describes the basic ‘mechanics’ of running the simulation, e.g. how to move the lance, how to make alloy additions, how to control oxygen flow, etc.

The underlying scientific relationships (chemistry, thermodynamics, reaction kinetics, etc.) that you will need to use in order to calculate alloy amounts, process parameters, etc. are presented in Section 8.

The common controls that are used include:

- **Stepper controls;** used for selecting amounts, these have up and down arrows which can be clicked on to increase or decrease the amount, or you can use the up and down arrow on your keyboard once the control has been selected.

7.1 Controls During Simulation

Once the simulation begins, different sources of information can be displayed and/or retrieved by pressing the relevant key given in the menu at the bottom left corner of the screen. For you convenience, these keys are:

A: Make Additions

C: View Steel Composition v Time

E: Event Log

P: View Melting Path (%C v Time)

R: Review / Request Analysis

S: View Slag Composition v Time

X: Close dialogue boxes

7.1.1 MAKE ADDITIONS (KEY A)

During the hot metal conversion, you can make iron ore, lime and dolomite additions. Each of these additives has a stepper control which is used to choose the amount to be added. By default all steppers are initially set to zero. The unit cost of each additive is displayed, together with the calculated cost for the selected amount.

TIP: Hover the cursor over the addition labels on the left for information about their composition and typical recovery rates.

Raw Material	Unit cost	Mass	Cost
Iron Ore			
Lime	\$85.00 / kg	1600 kg	136.00/kg
Dolomite	\$85.00 / kg	1750 kg	148.75/kg
Total:		3350 kg	\$284.75

Buttons: Clear, Cancel, Order

Figure 7-1: Screenshot illustrating the Addition interface. The boxed information shows the composition of Iron Ore used in the simulation.

Note that that additions made **do not** result in instantaneous changes to the steel composition, but take a finite time to dissolve. You can expect well-stirred additions made at higher temperatures to dissolve fast while additions at lower temperatures with little or no stirring will take many minutes to dissolve.

7.1.2 VIEW STEEL COMPOSITION VS. TIME (KEY C)

Pressing '**C**' on the keyboard displays a diagram of how the steel composition has changed over time. Elements displayed in this diagram include C, Si, Mn and P. This information might be vital for determining which additions to make and when.

At Works Technical level you will not be able to see this information during the simulation. However, it will be available at the summary screen so that it can be used as a part of a post-mortem.

7.1.3 VIEW EVENT LOG (KEY E)

The event log keeps a chronological record of all the major processing steps, including additions. This is useful for keeping track of what you have done so far during the simulation. It is also very useful in helping you analyze your results at the end of the simulation, as the log will often contain clues as to why you passed or failed the different criteria.

7.1.4 VIEW MELTING PATH (KEY P)

The melting path is a construction of information about carbon content, temperature and time during the simulation superimposed on a C-Fe phase diagram. Each dot represents one minute while the values of temperature and carbon content can be read out from the X- and Y-axis.

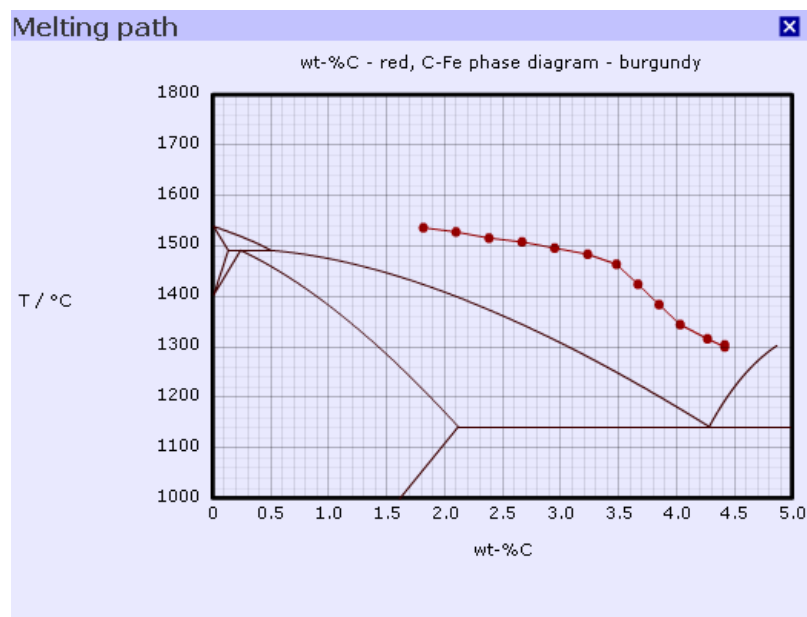


Figure 7-2: Screenshot of the Melting Path diagram, in which the carbon content and temperature as a function of time can be viewed.

Make sure that the melting path does not fall below the liquidus temperature, in which case the heat might become partially or fully solidified. Solidification of the heat results, of course, in failure.

7.1.5 VIEW OR REQUEST CHEMICAL ANALYSIS (KEY R)

You can view the most recent chemical analysis at any time by pressing key R. There is no cost penalty for this. In most cases, the steel chemistry will have changed since the last analysis was made. To initiate a new analysis, press the '**Take new sample**' button. The analysis

costs \$120, \$40 for the actual analysis and \$80 for the substance consumable part. The results take approximately 3 simulation minutes to arrive, e.g. about 22 real-world seconds if the simulation rate is set to $\times 8$.

The time at which the sample was taken is displayed near the top of the dialog box. You must always remember that the composition may have changed since the sample was taken.

7.1.6 VIEW SLAG COMPOSITION VS. TIME (KEY S)

Pressing '**S**' on the keyboard displays a diagram of how the slag composition has changed over time. Oxides displayed in this diagram include CaO, FeO_x, MnO, MgO and SiO₂. Primary use of this diagram is to determine which slag additions to make and when. Also, by following the FeO_x content in the slag, it is possible to conclude how best to choose the oxygen blowing pattern.

At Works Technical level you will not be able to see this information during the simulation. However, it will be available at the summary screen so that it can be used as a part of a post-mortem.

7.1.7 CLOSE DIALOG BOX(KEY X)

Press '**X**' closes any of these dialogue boxes.

7.2 Simulation Results

As soon as tapping has been completed, the simulation will end and the results of the heat displayed, together with the total operating costs, expressed as \$ per tonne.

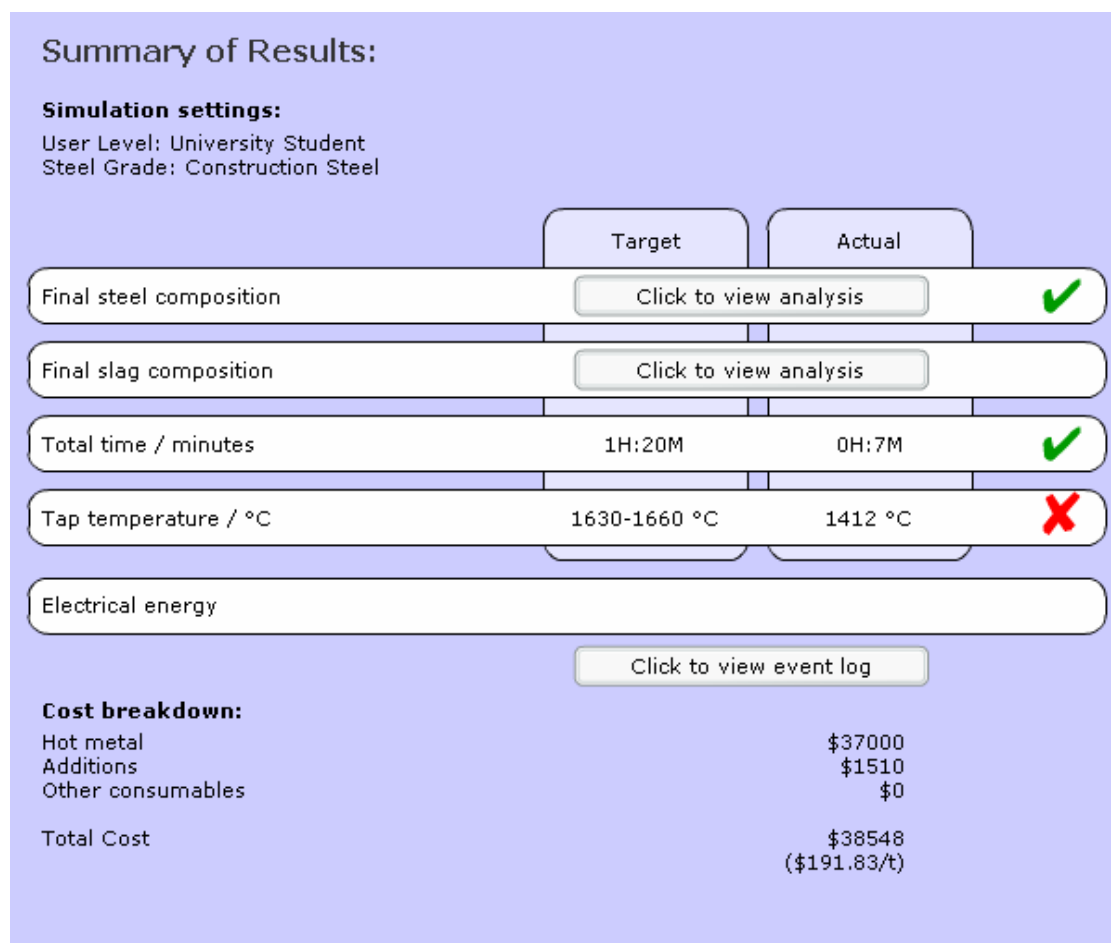


Figure 7-3: Screenshot of final results screen, in which the five criteria for success are displayed. Click on the "Event Log" button to help you analyze your results.

8 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.

8.1 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

8.1.1 ELEMENTAL ADDITIONS

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

$$m_{\text{additive}} = \frac{\Delta\% X \times m_{\text{steel}}}{100\%} \quad 8-1$$

where

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

m_{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?

$$m_{\text{additive}} = \frac{(1.0 - 0.01)\% \times 250,000 \text{ kg}}{100\%} = 2,475 \text{ kg} \quad 8-2$$

8.1.2 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 8-3:

$$\% X_{\text{steel, after}} = \frac{m_{\text{scrap}} \times \% X_{\text{scrap}} \times \text{recovery rate of } X + m_{\text{steel}} \times \% X_{\text{steel}}}{100 \times (m_{\text{scrap}} + m_{\text{steel}})} \quad 8-3$$

where

$\% X_i$ = content of element i in wt-%

m_{slag} = mass of slag in kg

m_{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 6-2), Heavy Scrap contains 0.05%C (Table 6-2) and carbon has got a 95% recovery rate (Table 6-3).

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

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.

8.1.3 MIXING TIMES

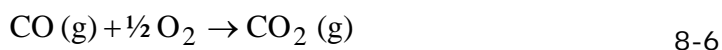
Note that that additions made **do not** result in instantaneous changes to the steel composition, but take a finite time to dissolve. In the simulation, be sure to allow sufficient time for additions to melt and dissolve by observing the following trends:

- 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.

8.2 Important Reactions

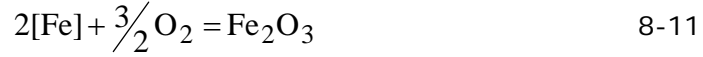
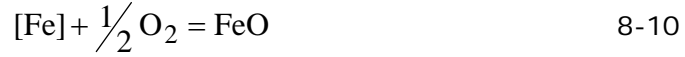
The hot metal charge is refined by rapid oxidation reactions on contact with the injected oxygen with the other elements present under conditions far removed from thermodynamic equilibrium. The three most important reactions are:



Post-combustion of CO into CO₂ (Equation 8-6) 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:





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).

8.2.1 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 8-1 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/SiO_2) of 3.

$$L_P = \frac{(\%P)_{\text{slag}}}{[\%P]_{\text{steel}}} \quad (\text{at equilibrium}) \quad 8-12$$

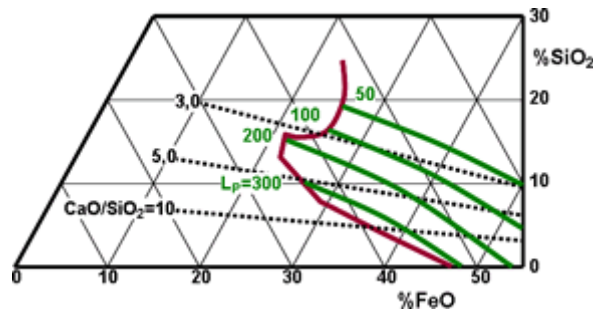


Figure 8-1: L_P in the system $\text{CaO-SiO}_2\text{-FeO-2\%P}_2\text{O}_5\text{-1.5\%Al}_2\text{O}_3\text{-3\%MnO-5\%MgO}$ at 1650 °C

8.2.2 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

$$\frac{d\%P}{dt} = k_c \times \frac{A}{V} \times [\%P - \%P_{\text{eq}}] = -\beta \times \sqrt{\frac{D_P \times Q}{A}} \times \frac{A}{V} \times [\%P - \%P_{\text{eq}}] \quad 8-13$$

where

k_c	=	mass transfer coefficient of P in molten steel
A	=	cross sectional area at the slag-metal interface (m^2)
V	=	steel volume (m^3)
$\%P$	=	P content in the steel at time t
$\%P_{eq}$	=	equilibrium P content at time t
β	=	empirical coefficient ($\sim 500 \text{ m}^{-1/2}$)
D_p	=	P diffusion coefficient in liquid steel ($\text{m}^2 \text{ s}^{-1}$)
Q	=	volumetric gas flow-rate across the interface ($\text{m}^3 \text{ s}^{-1}$)

8.2.3 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 8-2 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.

$$L_S = \frac{(\%S)_{\text{slag}}}{[\%S]_{\text{steel}}} \quad (\text{at equilibrium}) \quad 8-14$$

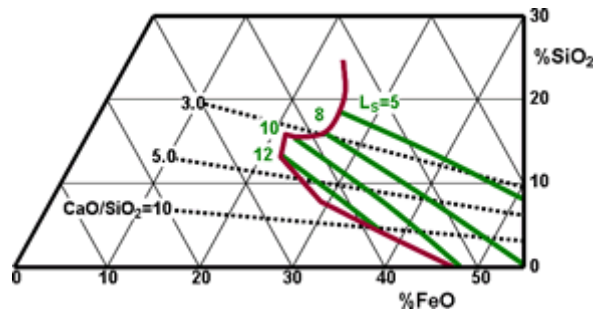


Figure 8-2: L_S in the system $\text{CaO-SiO}_2\text{-FeO-2}\%\text{P}_2\text{O}_5\text{-1.5}\%\text{Al}_2\text{O}_3\text{-3}\%\text{MnO-5}\%\text{MgO}$ at $1650\text{ }^\circ\text{C}$

8.2.4 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 $50\text{ }^\circ\text{C}$ leads to a decrease of L_{Mn} with a factor of ~ 1.25 .

$$L_{\text{Mn}} = \frac{(\% \text{Mn})_{\text{slag}}}{[\% \text{Mn}]_{\text{steel}}} \quad (\text{at equilibrium}) \quad 8-15$$

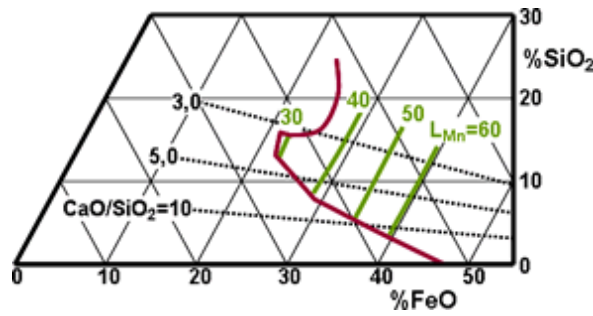


Figure 8-3: L_{Mn} in the system CaO-SiO₂-FeO-2%P₂O₅-1.5%Al₂O₃-3%MnO-5%MgO at 1650 °C

9 Writing Heat and Mass Balances

9.1 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

9.2 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.):

$$\sum \text{input} = \sum \text{output} (+ \text{losses}) \quad 9-1$$

One can consider:

- global balances
- balance for certain entities (gas, slag, etc.)
- elementary balances (Fe, O₂, CaO, etc.)

For instance, the balance for element X is written:

$$\frac{1}{100} \sum_i Q_{E_i} \cdot \% X_{E_i} = \frac{1}{100} \sum_j Q_{S_j} \cdot \% X_{S_j} (+ \text{losses}) \quad 9-2$$

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.

9.3 Heat Balance

9.3.1 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 :

$$H_{T_2} - H_{T_1} = \int_{T_1}^{T_2} C_p \cdot dT \quad 9-3$$

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.

9.3.2 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:

$$\Delta H_1 + \Delta H_R + \Delta H_2 + \text{heat loss} = 0 \quad 9-4$$

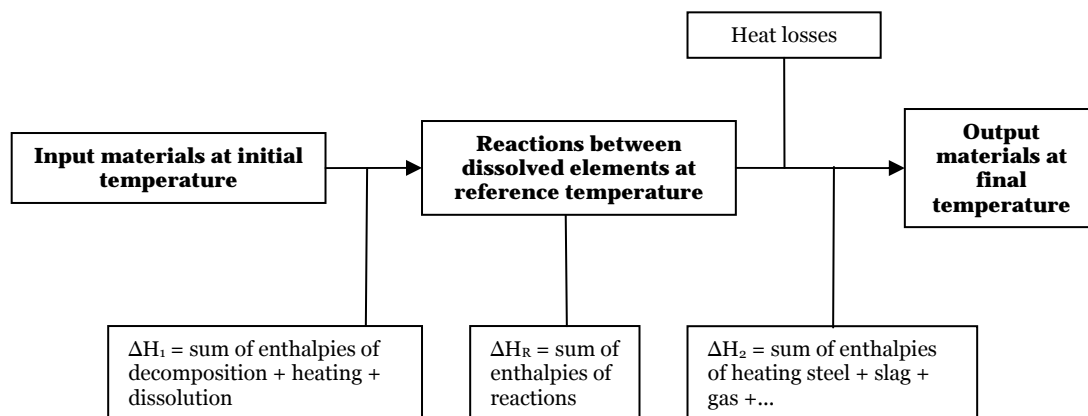


Figure 9-1: Calculation scheme for a heat balance.

The data in Tables 9.1 to 9.4 are used to compute the terms ΔH_1 , ΔH_2 and ΔH_R . The values of ΔH_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 ΔH_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 :

$$\Delta T_{\text{steel}} = \frac{\Delta H_2}{0.82 Q_{\text{steel}} + 2.04 Q_{\text{slag}}} \quad 9-5$$

where

ΔH_2 = sum is of heating enthalpies in MJ

Q_{steel} = mass of steel in tonnes

Q_{slag} = mass of slag in tonnes

Table 9-1: Enthalpy values for materials as a function of temperature.

	$H (1400\text{ °C}) - H (25\text{ °C})$		$C_p \text{ at } 1400\text{ °C}$	
	/ MJ kg⁻¹		/ kJ K⁻¹ kg⁻¹	
Hot metal (liquid at 1400 °C)	1.30 to 1.37		0.87	
	$H (1600\text{ °C}) - H (25\text{ °C})$		$C_p \text{ at } 1600\text{ °C}$	
	/ MJ kg⁻¹		/ kJ K⁻¹ kg⁻¹	
Low-alloyed steel (liq at 1600 °C)	1.35		0.82	
Refining slag (liq at 1600 °C)	2.14		2.04	
Iron ore Fe ₂ O ₃ (=> Fe _{liq} + Q)	4.43			
CaO	1.50		1.03	
	$H (1600\text{ °C}) - H (25\text{ °C})$		$C_p \text{ at } 1600\text{ °C}$	
	/ MJ kg⁻¹	/ MJ m⁻³	/ kJ K⁻¹ kg⁻¹	/ kJ K⁻¹ m⁻³
Ar	0.82	1.46	0.53	0.93
CO	1.86	2.33	1.28	1.61
CO ₂	1.90	3.78	1.36	2.71
N ₂	1.84	2.30	1.28	0.95
O ₂	1.70	2.43	1.17	1.68

Table 9-2: Enthalpy of oxidation reactions for various elements.

Element X to Oxide X_nO_m	Heating from 25 to 1600 °C + dissolution / MJ kg ⁻¹	C_p element X at 1600 °C / kJ K ⁻¹ kg ⁻¹	Oxidation X at 1600 °C by dissolved O / MJ kg ⁻¹	Oxidation X at 1600 °C by O ₂ gas at 25 °C / MJ kg ⁻¹	Amount O ₂ / kg / m ³	
C in CO	4.56* to 6.0**	2.025	-1.93* to -3.37**	-9.4* to -10.84**	1.33	0.93
C in CO₂	4.56* to 6.0**	2.025	-15.35* to -16.79**	-30.35* to - 31.79**	2.67	1.87
Al in Al₂O₃	- 0.17	1.175	- 22.32	- 27.32	0.89	0.62
Cr in Cr₂O₃	1.37	0.95	- 7.76	- 10.36	0.46	0.32
Fe in "FeO" liq	1.35	0.82	- 2.49	- 4.10	0.29	0.20
Fe in Fe₂O₃	1.35	0.82	- 4.06	- 6.48	0.43	0.30
Mn in MnO	1.53	0.835	- 5.34	- 6.97	0.29	0.20
P in C₃P***	- 0.14	0.61	- 23.8	- 31.05	1.29	0.90
Si in C₂S***	- 1.43	0.91	- 24.4	- 29.35	1.14	0.80

(*) in liquid steel

(**) in hot metal

(***) to form 3 CaO-P₂O₅ and 2 CaO-SiO₂ with necessary CaO taken at 1600 °CTable 9-3: Reactions of oxygen dissolution in liquid steel at 1600 °C (MJ/kg O₂).

From O ₂ gas at 25 °C	From FeO _x in slag at 1600 °C	From very stable oxides at 1600 °C
- 5.62	8.7	18

Table 9-4: Enthalpy of decomposition of ferroalloys at 25°C (MJ/kg alloy).

High C Ferro-Cr (64%Cr 5%C)	Refined Ferro-Cr (73%Cr 0.5%C)	High C Ferro-Mn (78%Mn 7%C)	Refined Ferro-Mn (80%Mn 1.5%C)	Ferro- Silicon (75%Si)	Ferro- Silicon (50%Si)	Silico- Manganese (35%Si)
0.11	- 0.025	0.10	0.075	0.37	0.70	0.71

9.3.3 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 (+ O₂ gas) per tonne of steel?

Applying the heat balance shown in Equation 9-4 provides the necessary parameters.

The materials balance indicates that 0.89 kg O₂ are necessary per kg Al, and that 1.89 kg Al₂O₃ are formed (see Table 9-2).

1. Calculation of ΔH_1 : - 5.13 MJ including:
 - a. Heating and dissolution of 1 kg Al:
 - i. - 0.17 MJ (heating at 1600 °C + dissolution, see Table 9-2)
 - ii. + 1.175.10⁻³×20 (heating from 1600 to 1620 °C)
 - b. Heating and dissolution of 0.89 kg O₂ :
 - c. - 5.62×0.89 MJ (heating at 1600 °C + dissolution, see Table 9-3)
 - d. +1.17.10⁻³×20×0.89 (heating from 1600 to 1620 °C)
2. Calculation of ΔH_R : -22.32 MJ (see Table 9-2)
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 Al_2O_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 ΔH_1 the enthalpy of dissolution of oxygen, i.e. $(-5.62 \times 0.89 \text{ MJ/kg Al})$. 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 ΔH_1 the enthalpy of decomposition of FeO_x , i.e. $(8.7 \times 0.89 \text{ MJ/kg Al})$. In this case, the temperature change would be:

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

10 Charge Calculation

10.1 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 CO_2) 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 $PCR = \text{CO}_2 / (\text{CO} + \text{CO}_2)$ where CO and CO_2 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 $O_{\text{linked}} \text{ to Fe} / \text{Fe}_{\text{oxidized}} = 0.33$.

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 oxidized 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 $(\text{CaO}+\text{MgO})/(\text{SiO}_2+\text{P}_2\text{O}_5)$, 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 10-1: Input and Output material from the Basic Oxygen Steelmaking Process.

Input	Hot metal	Weight fixed (or unknown) (P_{Fte}), composition and temperature fixed
	Scrap or Ore	Weight unknown (P_{Fer} or P_{M}), composition and temperature fixed
	Burnt lime	Weight unknown (P_{Chx}), composition and temperature fixed
	Oxygen	Weight unknown (P_{O}), composition and temperature fixed
Output	Liquid steel	Weight unknown (or fixed) (P_{A}), composition and temperature fixed
	Slag	Weight unknown (P_{L}), temperature fixed Iron oxide and oxidation degree fixed ($=> \% \text{Fe}_\text{L}$, $(\% \text{O}_{\text{Fe}})_\text{L}$) Complete composition will be computed from elementary balances (Si, P, etc.)
	Gas	Weight unknown (P_{G}) Average temperature and post-combustion ratio (PCR) fixed

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

10.2 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:

$$z = \sum_j c_j \cdot P_j \quad 10-1$$

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.:

$$\sum_{j=1}^n a_{ij} \cdot P_j \{ \leq, =, \geq \} b_i \quad i = 1, \dots, m \quad 10-2$$

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).

10.3 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.

10.3.1 FE BALANCE

$$[\%Fe_{Fte} \cdot P_{Fte} + \%Fe_{Fer} \cdot P_{Fer} + \%Fe_M \cdot P_M] = [\%Fe_A \cdot P_A + \%Fe_L \cdot P_L] \quad 10-3$$

10.3.2 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} .

$$Q_C = 0.01 \cdot [\%C_{Fte} \cdot P_{Fte} + \%C_{Fer} \cdot P_{Fer} - \%C_A \cdot P_A] \quad 10-4$$

(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:

$$\begin{aligned} P_O + 0.01 \cdot \%O_M \cdot P_M = & \left[\frac{16}{12} \cdot (1 - PCR) + \frac{32}{12} \cdot PCR \right] \cdot Q_C + \frac{16}{55} \cdot Q_{Mn} \\ & + \frac{80}{62} \cdot Q_P + \frac{32}{28} \cdot Q_{Si} + 0.01 \cdot (\%O_{Fe})_M \cdot P_L + 0.01 \cdot \%O_A \cdot P_A \end{aligned} \quad 10-5$$

10.3.3 GAS BALANCE

$$P_G = \left[\frac{28}{12} \cdot (1 - TCS) + \frac{44}{12} \cdot (TCS) \right] \cdot Q_C \quad 10-6$$

When using a stirring gas (Ar, N₂, etc.), it is necessary to add P_{Ar} , P_{N_2} , etc.

10.3.4 BALANCE OF SLAG ELEMENTS OTHER THAN FE

$$\begin{aligned} \frac{71}{55} \cdot Q_{Mn} + \frac{142}{62} \cdot Q_P + \frac{60}{28} \cdot Q_{Si} + 0.01 \cdot \%CaO_{Chx} \cdot P_{Chx} \\ = 0.01 \cdot [100 - \%Fe_L - (\%O_{Fe})_L] \cdot P_L \end{aligned} \quad 10-7$$

10.3.5 BASICITY EQUATION

If, for instance, the basicity ratio $v = \%CaO/\%SiO_2$ is imposed:

$$0.01 \cdot \%CaO_{Chx} \cdot P_{Chx} = v \cdot \frac{60}{28} \cdot Q_{Si} \quad 10-8$$

10.3.6 ENERGY BALANCE

We use Equation 9-4 of section **9.3 Heat Balance**, taking 1600 °C for reference so that the data of Tables 9-1 to -9.4 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)

$$\begin{aligned} \Delta H_1 = & 0.00087 (1600 - T_{Fte}) P_{Fte} && \text{(heating hot metal - see Table 9-1-)} \\ & + 1.35 P_{Fer} + 4.43 P_M && \text{(heating and dissolving scrap and ore - see Table 9-1-)} \\ & + 1.5 P_{Chx} && \text{(heating burnt lime - see Table 9-1-)} \\ & - 5.62 P_O && \text{(heating and dissolving oxygen - see Table 9-3-)} \end{aligned}$$

Also use data from Table 9-4 and the first column of Table 9-2 if ferroalloys are being charged.

Step 2

Enthalpy of reactions between dissolved elements at 1600 °C (Table 9-2).

$$\begin{aligned} \Delta H_2 = & [-3.37 \cdot (1 - PCR) - 16.79 \cdot PCR] \cdot Q_C \\ & - 5.34 \cdot Q_{Mn} - 23.8 \cdot Q_P - 24.4 \cdot Q_{Si} - 0.0296 \cdot \%Fe_L \cdot P_L \end{aligned} \quad 10-9$$

Step 3

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

$$\begin{aligned} \Delta H_3 = & 0.00082 (T_A - 1600) P_A && (\Delta T_{steel} - \text{see Table 9-1}) \\ & + 0.00204 (T_L - 1600) P_L && (\Delta T_{slag} - \text{see Table 9-1}) \\ & + [\{0.00128 (T_G - 1600)\} (1 - PCR) + \{0.00136 (T_G - 1600)\} PCR] Q_C \\ & && (\Delta T_{gas} \text{ for CO + CO}_2 - \text{see Table 9-1}) \end{aligned}$$

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

$$+\{0.82+0.00053 (T_G-1600)\} P_{Ar}+\{1.84+0.00128 (T_G-1600)\} P_{N_2}$$

Table 10-2: Starting values for the heat and mass balance.

Hot metal composition	4.5 %C, 0.5 %Mn, 0.08 %P, 0.4 %Si (that is 94.52 %Fe) at 1350 °C.
Scrap composition	100 %Fe. – No ore.
Burnt lime	100 %CaO.
Liquid steel composition	0.05 %C, 0.12 %Mn, 0.01 %P (that is 99.73 %Fe) at 1650 °C.
Slag	%CaO/%SiO ₂ =4, oxidized Fe content 18% at 1650 °C.
Gas	PCR=0.08 extracted at an average temperature of 1500 °C.
Heat losses	65 MJ/t steel.

10.4 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:

$$Q_C = 0.045 P_{Fte}-0.5$$

$$Q_{Mn} = 0.005 P_{Fte}-1.2$$

$$Q_P = 0.0008 P_{Fte}-0.1$$

$$Q_{Si} = 0.004 P_{Fte}$$

Then, all 6 heat and mass balance equations are calculated according to Table 10-3:

Table 10-3: Heat and Mass balance end equations.

Fe balance	$0.9452 \cdot P_{Fte} + P_{Fer} - 0.18 \cdot P_L = 997.30$
O balance	$0.0718 \cdot P_{Fte} + P_O + 0.0544 \cdot P_L = 1.098$
Gas balance	$0.1098 \cdot P_{Fte} - P_G = 1.22$
Balance of slag elements other than Fe	$0.0169 \cdot P_{Fte} + P_{Chx} - 0.7606 \cdot P_L = 1.778$
Slag basicity	$0.0343 \cdot P_{Fte} - P_{Chx} = 0$
Energy balance	$-0.1287 \cdot P_{Fte} + 1.35 \cdot P_{Fer} + 1.5 \cdot P_{Chx} - 5.62 \cdot P_O - 0.3462 \cdot P_L = -117.2$

Finally, the masses are calculated:

$$P_{Fte} = 885.3 \text{ kg}$$

$$P_{Fer} = 171.6 \text{ kg}$$

$$P_{Chx} = 30.4 \text{ kg}$$

$$P_O = 65.6 \text{ kg}$$

$$P_A = 1000 \text{ kg}$$

$$P_L = 57.2 \text{ kg}$$

$$P_G = 96.0 \text{ kg}$$

11 Bibliography

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