Application Example:

Using the Process Metallurgy Module to Calculate the Basic Oxygen Furnace (BOF) Process: using Equilibrium Calculations

Database(s):	**TCOX9 or OXDEMO**	Module(s):	**Process Metallurgy Module (PMM)**
Material/Application:	**Basic oxygen furnace Steelmaking**	Calculator(s):	
Version required:	**Thermo-Calc 2019b or newer**		
Example file:	https://www.thermocalc.com/solutions/example-calculations/basic-oxygen-furnace-process/		

To run the calculation, download the example file[1], save it to your computer, then double click on it. The calculation will open in Thermo-Calc if you have Thermo-Calc installed on your computer and licenses for all databases[2]and modules listed above.

INTRODUCTION

Thermo-Calc Software offers two application examples showing how the Process Metallurgy Module can be used to calculate the Basic Oxygen Furnace Process. This example uses equilibrium calculations to gain a general understanding of your BOF process and help you determine optimal operation conditions and predict and optimize costs of raw materials and recycling. The other example gives detailed instructions on how to simulate the kinetics of the Basic Oxygen Furnace Process using the kinetic process simulation released in Thermo-Calc 2020b.

Steelmaking in a basic oxygen furnace (BOF)

In very simple terms, the principle of oxygen steelmaking is to blow oxygen into the carbon-rich hot metal (typical carbon content is about 4.5 wt%) coming from a blast furnace. The oxygen combines with the dissolved carbon to form CO which escapes as a gas phase. The hot metal is thereby transformed into liquid steel with low carbon content.

[1] This example includes two calculation files, one if you have a license for the database TCOX9 or newer, and a simplified example that can be run using the OXDEMO database included in all Thermo-Calc installations.
[2] You do not need the database version(s) that are listed, but results from other versions may vary slightly.

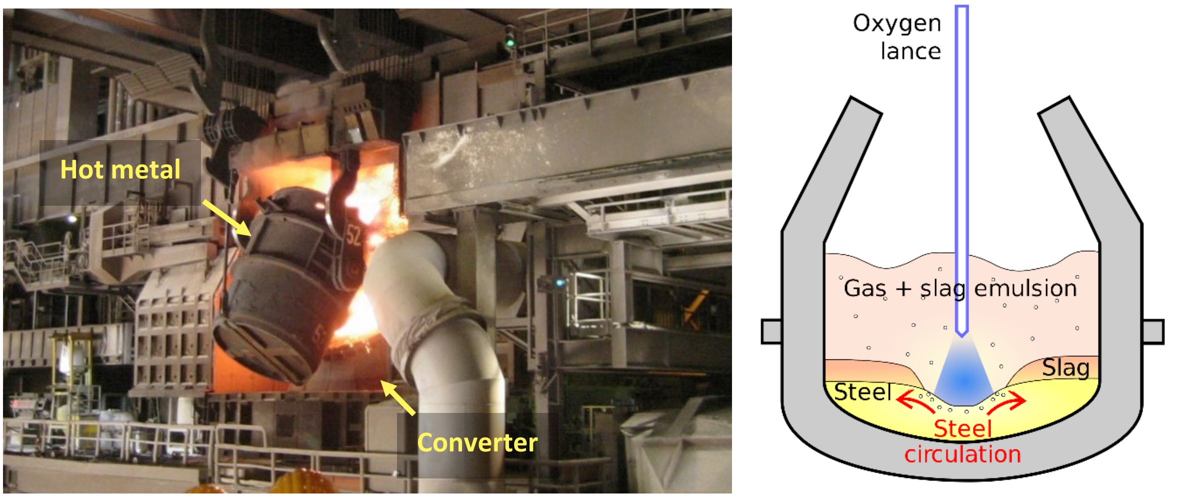

Figure 1. Hot metal being charged into the BOF converter (left) and schematic principle of operation of a basic oxide converter (BOF) *(Images by Katpatuka, CC BY-SA 3.0, commons.wikimedia.org/w/index.php?curid=11903007)*

The reaction of dissolved carbon with oxygen is highly exothermic and the temperature of the liquid increases dramatically during the process. In fact, the temperature increases so much that cooling scrap must be added to the converter to prevent the temperature from going above the aim temperature of ~1700°C at the end of the blowing process.

Apart from the removal of carbon from the hot metal, there are many other reactions that occur simultaneously.

Two elements that are very important in steelmaking and steel refining are S and P. Both of these elements are usually undesirable and must be removed from the liquid steel. This is usually done by transferring them to a CaO-rich slag phase by the following reactions:

$$2[P] + 5[O] + 4(CaO) \rightarrow (4CaO \cdot P_2O_5) \qquad \textit{Eq. 1}$$

$$2[P] + 5(Fe_tO) + n(CaO) \rightarrow (nCaO \cdot P_2O_5) + 5[Fe_t] \qquad \textit{Eq. 2}$$

$$(CaO) + [S] \rightarrow 2(CaS) + [O] \qquad \textit{Eq. 3}$$

Round brackets () indicate elements dissolved in the slag phase and square brackets [] indicate elements dissolved in the liquid steel phase. Inspecting the reactions above, it is seen that P is transferred to the slag phase under *oxidizing* conditions, whereas S is transferred to the slag under *reducing* conditions. As large amounts of oxygen are blown into the BOF, it is obvious that the conditions will be oxidizing. Therefore, it is expected that conditions might be suitable to remove P from the liquid metal, but S probably cannot be removed. This question will be examined in this example.

EXAMPLE SET-UP: BASIC OXYGEN FURNACE

Example files: Ex-4a-BOF_DEMO.tcu, Ex-4b-BOF_TCOX.tcu

Another version of this example is packaged with Thermo-Calc 2020b and newer (Help → Example Files… → Process Metallurgy → PMET_01_Basic_Oxygen_Furnace.tcu) and there is also a video demonstrating the setup of that example at https://www.youtube.com/playlist?list=PLfv6McToaTGS4g5LC9tjiqjCo9OX2-YOa. We used this standard example as basis for the examples outlined here.

The screenshot of the Process Metallurgy Module shown in Figure 2 shows how to set up the calculation. We assume the process is isothermal at 1650°C (1). We change the composition of the hot metal compared to the standard example by adding 0.08 wt% S and 0.06 wt% P (2), in order to investigate how the concentration of these elements changes during the blowing process. We perform two simulations: in the first simulation we add no slag (3), in the second we add 3 t of a slag containing 75% CaO and 25% Al2O3 (4). As in the standard example, we perform a one axis calculation, stepping from 0 to 7000 Nm3 Oxygen to simulate the blowing process (5).

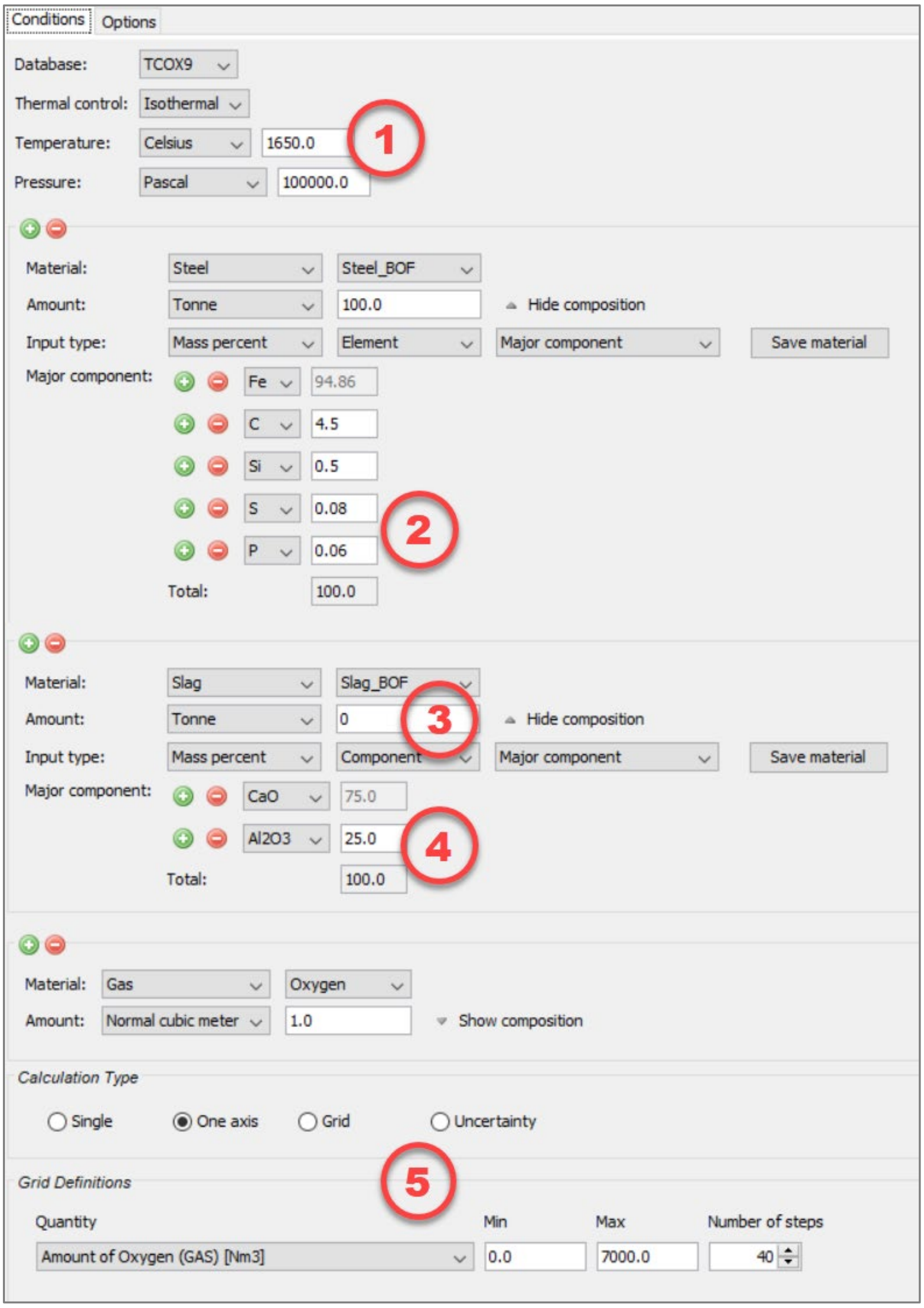

Figure 2. Screenshot of the Process Metallurgy Module in Thermo-Calc showing how to set up the basic oxygen furnace example.

EXAMPLE RESULTS

Figure 3 shows how the liquid steel chemistry changes as a function of amount of oxygen blown into the system. The plot on the left is the calculation without slag. While the carbon content is reduced as desired (red line), there is no change in the P content of the steel (light blue line). The plot on the right is calculated with 3t of slag added. With the slag, the P content is reduced (light blue line) during the end of the blow as it is transferred to the slag phase according to Eq. 1 and Eq. 2.

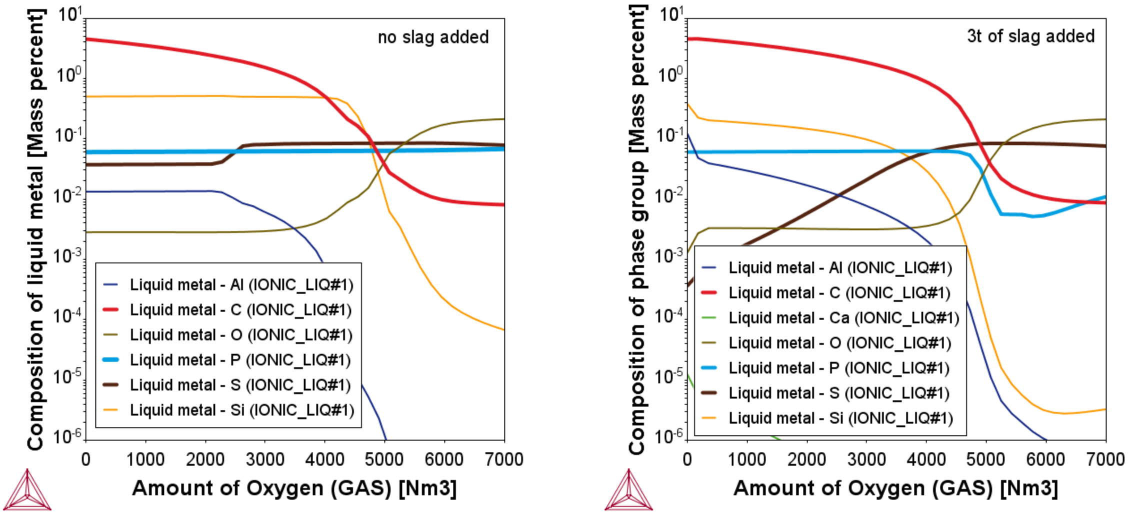

Figure 3. Change of the chemical composition of the liquid metal as a function of added oxygen. In the left plot, no slag formers are added. In the right plot, 3t of CaO rich slag formers are added, leading to a reduction in P content during the end of the blow, as shown by the light blue line.

Many other properties of the system can be plotted. For example, the amounts of phases and the composition of the slag phase (Figure 4).

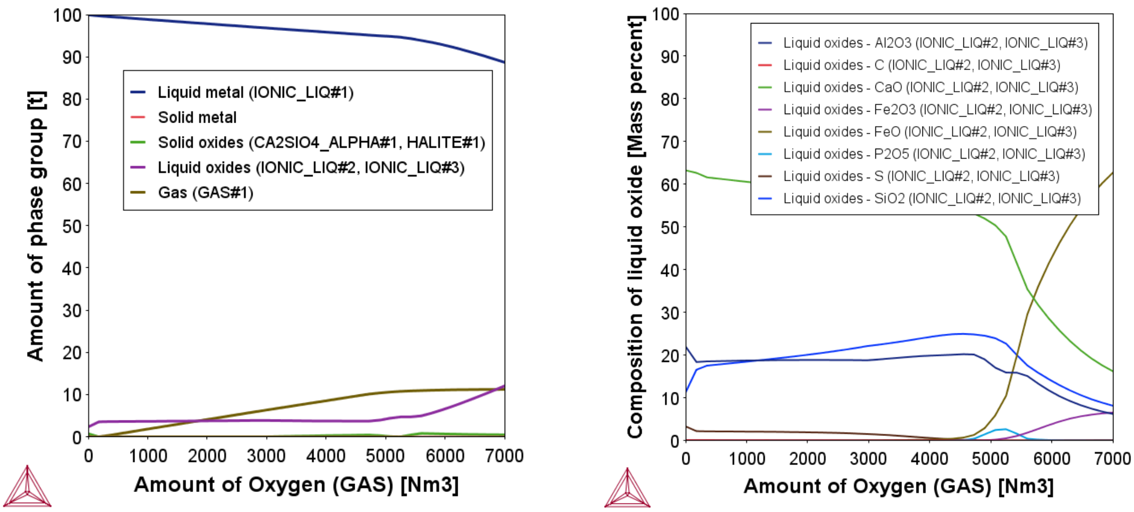

Figure 4. Changes of the amounts of the various phases (liquid metal, liquid oxides and gas phase) as a function of added oxygen (left) and composition of the liquid slag phase (right).

By performing a two axis grid calculation, an optimum combination of amount of oxygen and amount of slag required to remove both C and P from the liquid steel can be obtained for a given hot metal and slag composition (see Figure 5, left plot). In this case, about 5500 Nm3 of oxygen needs to be blown and about 2.7 t of high CaO slag former must be added.

The plot on the right shows that, after the steelmaking process, about 5t of oxide slag is formed (blue contour lines, so 2.3 t more than was originally added). The additional oxides come from oxidized components of the steel such as Si. Furthermore, significant amounts of Fe are oxidized to FeO, thereby reducing the yield of the process. At the end of the process, the liquid steel contains about 1000 ppm dissolved oxygen (red contour lines). Such a calculation thus not only predicts the amount of raw materials required (left plot) but also the amount of waste produced and the yield of the process. Knowing the cost of the raw materials and the cost of recycling[3] the produced slag allows a calculation and optimization of the total cost of the converter process.

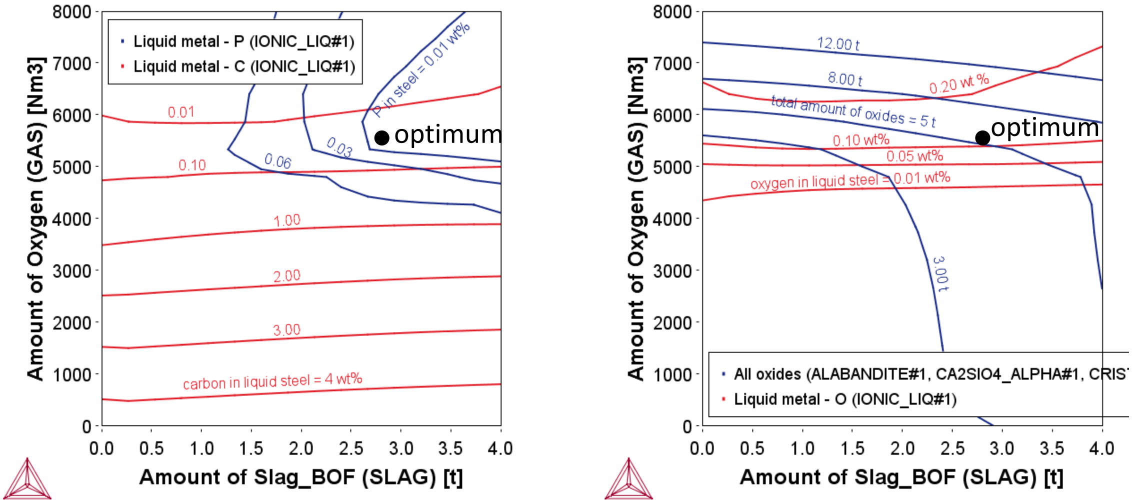

Figure 5. Carbon and Phosphorous content in liquid metal (left) and total amount of oxide phases and oxygen content in the liquid metal (right) as a function of oxygen and slag phase added to the system. The optimal combination is shown as a black dot.

KINETICS OF THE STEELMAKING PROCESS

This calculation assumed that the whole system (all the hot metal and slag in the converter and also the O2 -gas being added) is in thermodynamic equilibrium. While this is certainly not the case in reality, such an equilibrium calculation gives important information on where the reactions in the converter are heading. In the near future, a kinetic model will be introduced to the Process Metallurgy module that will also include reaction kinetics.

Including kinetics would allow the calculation to be performed under adiabatic conditions in order to simulate the typical temperature increase from ~1300°C to ~1700°C during the blowing process. Performing an equilibrium calculation under adiabatic conditions results in the temperature reaching unreasonably high values of > 2000°C due to the fact that it is not possible to simulate the heat lost due to radiation / convection and also it is not possible to properly consider the addition of cooling scrap.

[3] In most plants the BOF slag is recycled by charging it into the blast furnace, where the oxidized iron (FeO) is recovered.