

Application Example:

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

Database(s):	TCOX11 or newer, OXDEMO	Module(s):	Process Metallurgy Module
Version required:	Thermo-Calc 2021b or newer	Calculator(s):	Equilibrium
Material/Application:	Steelmaking / Basic oxygen furnace		
Calculation name:	PMET_01_Basic_Oxygen_Furnace		

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.

How to Run the Calculation

To run the calculation, open Thermo-Calc and navigate to the Help Menu → Example Files... → Process Metallurgy. This example includes tree calculation files:

- **PMET_01a_Basic_Oxygen_Furnace:** works with the free Educational Package and the OXDEMO database.
- **PMET_01b_Basic_Oxygen_Furnace:** can be run with the OXDEMO database but requires a full license for Thermo-Calc 2021b or newer.
- **PMET_01c_Basic_Oxygen_Furnace:** requires a full license for Thermo-Calc 2021b or newer, the Metal Oxide Solutions Database TCOX11 or newer, and a license for the Process Metallurgy Module.



There is also a [video demonstrating the setup of PMET_01b](#).



Read additional in-depth [Application Examples available for the Process Metallurgy Module](#), which discuss topics such as Steel Deoxidation on Tapping and Kinetics of Steel Refining in a Ladle Furnace.

Steelmaking in a Basic Oxygen Furnace (BOF)

In 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.

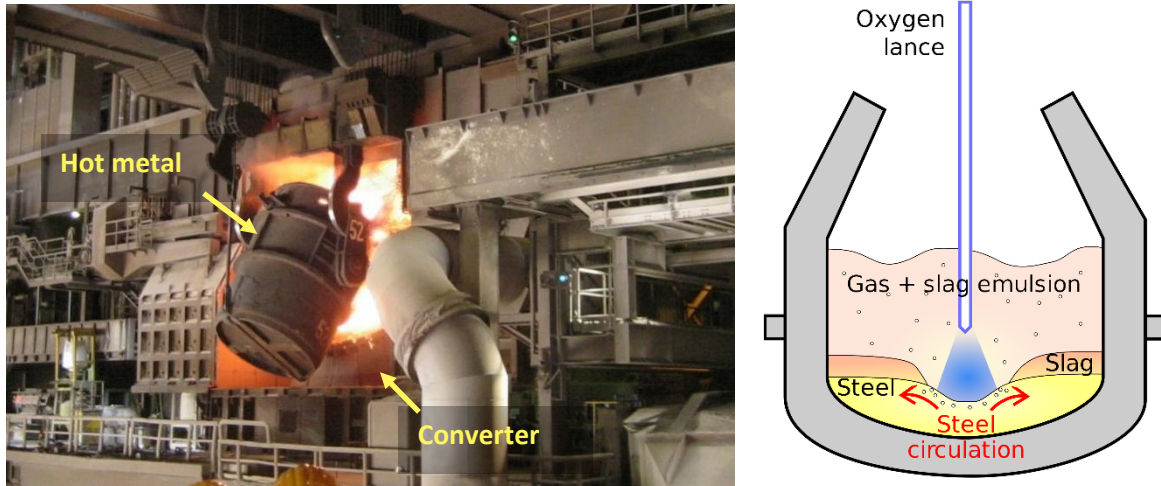
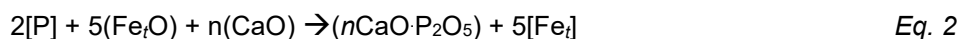


Figure 1. Hot metal being charged into the BOF converter (left) and schematic principle of operation of a basic oxide converter (BOF) (Images by Katpatuka, CC BY-SA 3.0, commons.wikimedia.org/w/index.php?curid=11903007)

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.

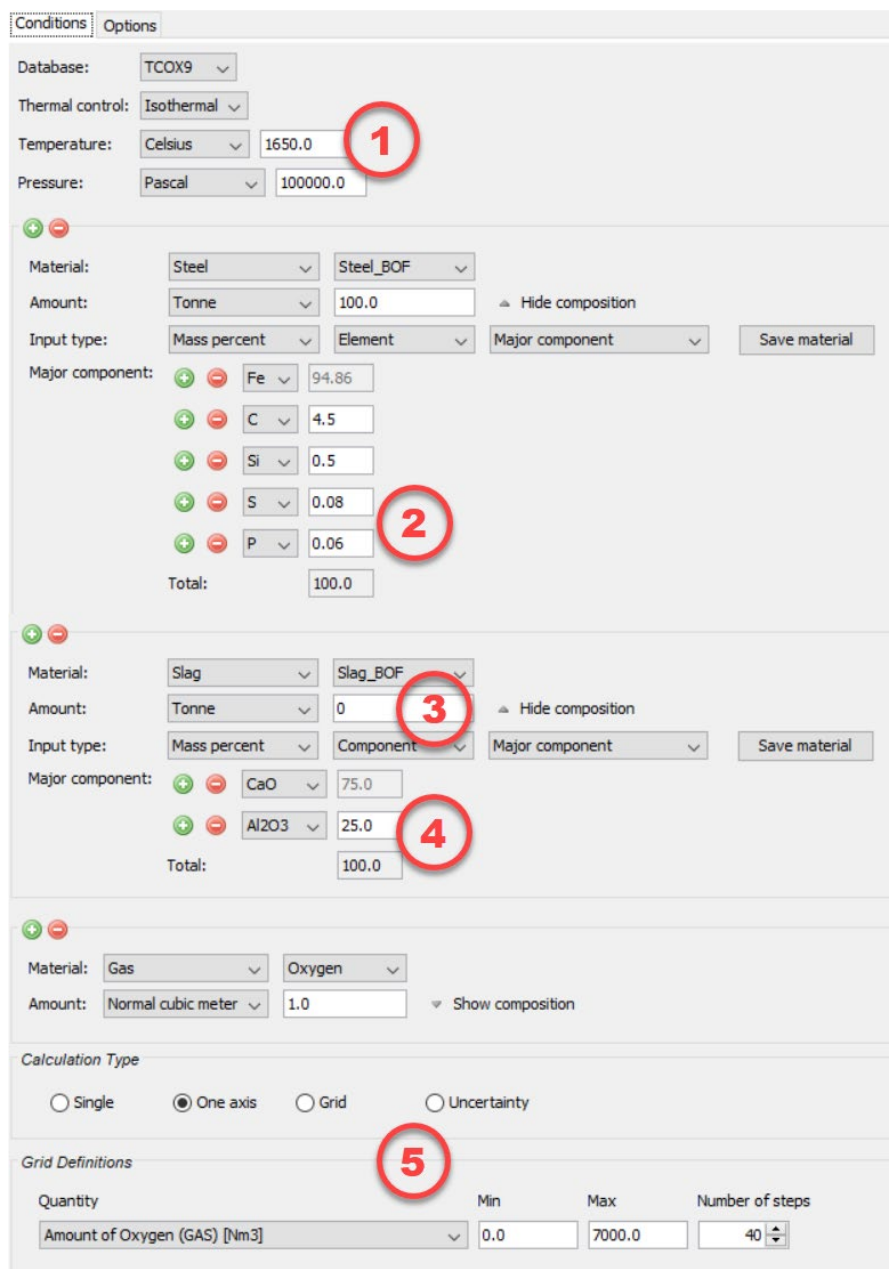
Two elements that are very important in steelmaking and steel refining are S and P. Both of these elements are usually undesirable and must be removed from the liquid steel. This is usually done by transferring them to a CaO-rich slag phase by the following reactions:



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 is examined in this example.

EXAMPLE SET-UP: BASIC OXYGEN FURNACE

Only the results of the example 1c, calculated with the full version of Thermo-Calc and the TCOX11 database, are discussed in the following. Newer versions of the database result in virtually identical results. 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 change 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).



The screenshot shows the following configuration in the Process Metallurgy Module:

- Conditions:** Database: TCOX9; Thermal control: Isothermal; Temperature: Celsius, 1650.0; Pressure: Pascal, 100000.0.
- Options:**
 - Material:** Steel, Steel_BOF; Amount: Tonne, 100.0; Input type: Mass percent, Element; Major component: Fe (94.86), C (4.5), Si (0.5), S (0.08), P (0.06); Total: 100.0.
 - Material:** Slag, Slag_BOF; Amount: Tonne, 0; Input type: Mass percent, Component; Major component: CaO (75.0), Al2O3 (25.0); Total: 100.0.
 - Material:** Gas, Oxygen; Amount: Normal cubic meter, 1.0.
- Calculation Type:** Single, One axis, Grid, Uncertainty.
- Grid Definitions:** Quantity: Amount of Oxygen (GAS) [Nm3]; Min: 0.0; Max: 7000.0; Number of steps: 40.

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 (light blue line), there is no change in the P content of the steel (green line). The plot on the right is calculated with 3 t of slag added. With the slag, the P content is reduced (green line) during the end of the blow as it is transferred to the slag phase according to [Eq. 1](#) and [Eq. 2](#).

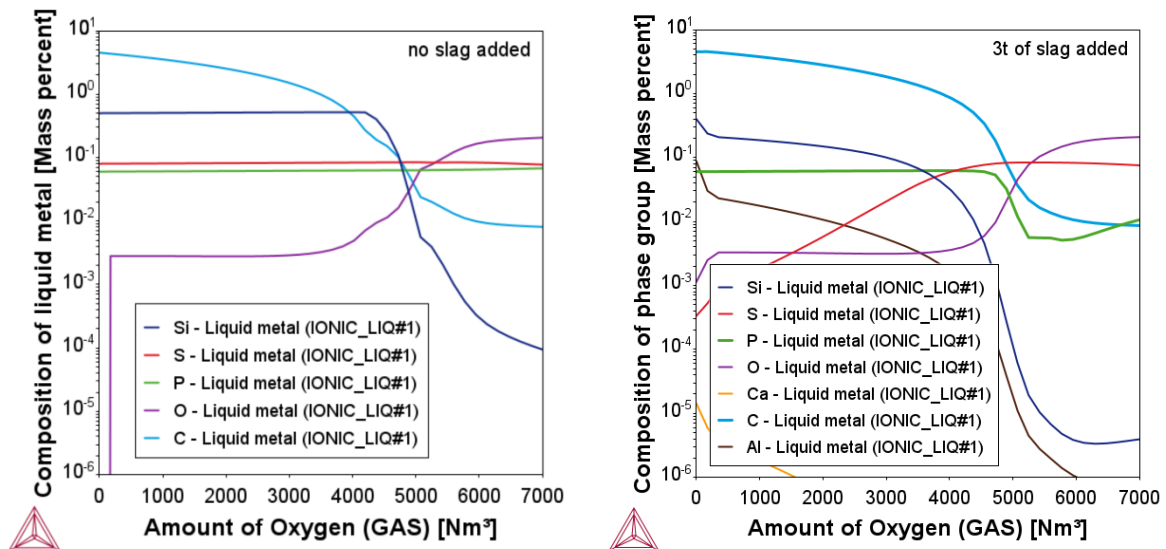


Figure 3. Change of the chemical composition of the liquid metal as a function of added oxygen. In the left plot, no slag formers are added. In the right plot, 3 t of CaO rich slag formers are added, leading to a reduction in P content during the end of the blow, as shown by the green line.

Many other properties of the system can be plotted. For example, the amounts of phases (Figure 4) and the composition of the slag phase (Figure 5).

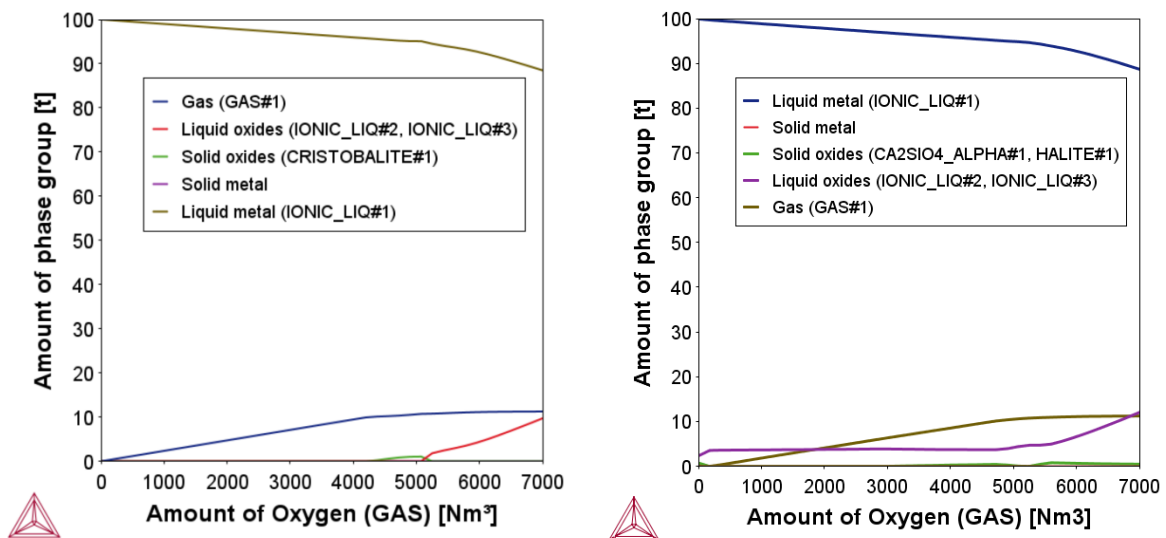


Figure 4. Changes of the amounts of the various phases (e.g., liquid metal, liquid oxides, and gas phase) as a function of added oxygen with no slag formers added (left), and with 3 t of CaO rich slag formers are added (right).

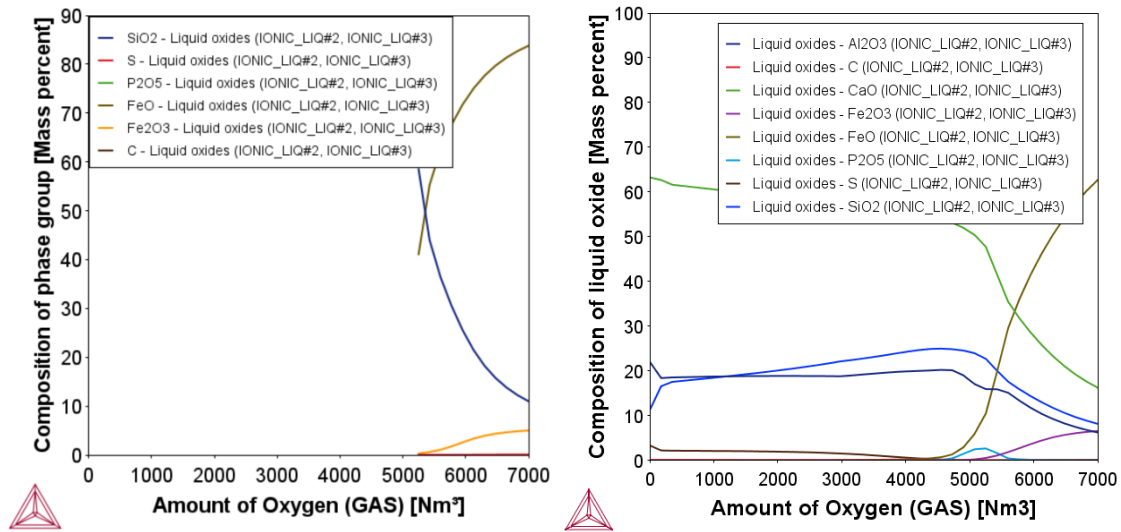


Figure 5. Composition of the liquid slag phase as a function of added oxygen with no slag formers added (left), and with 3 t of CaO rich slag formers are added (right).

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 6, 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 5 t 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 recycling¹ the produced slag allows a calculation and optimization of the total cost of the converter process.

¹ In most plants the BOF slag is recycled by charging it into the blast furnace, where the oxidized iron (FeO) is recovered.

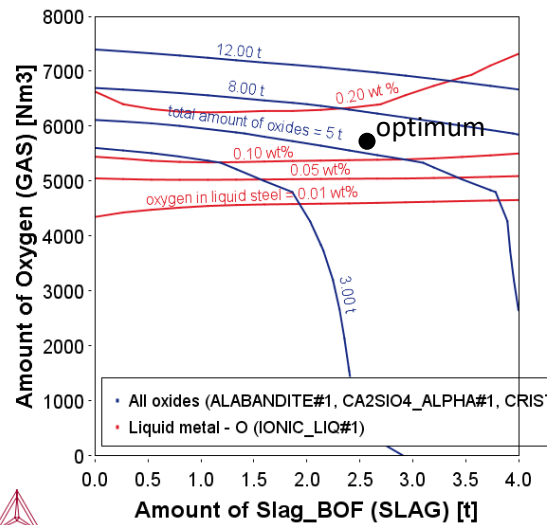
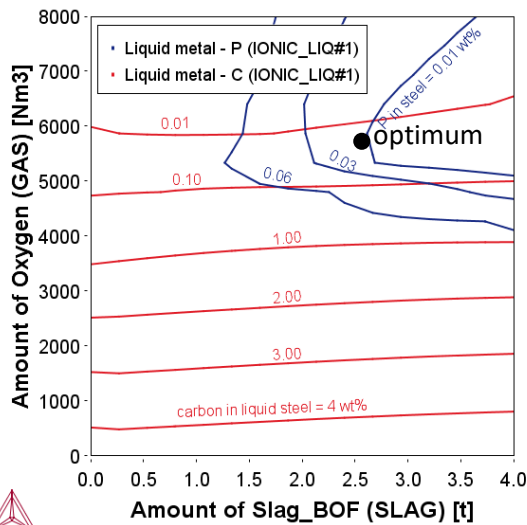


Figure 6. Carbon and phosphorous content in liquid metal (left) and total amount of oxide phases and oxygen content in the liquid metal (right) as a function of oxygen and slag phase added to the system. The optimal combination is shown as a black dot.

KINETICS OF THE STEELMAKING PROCESS

This calculation assumes that the whole system (all the hot metal and slag in the converter and also the O_2 -gas being added) is in thermodynamic equilibrium. While this is certainly not the case in reality, such an equilibrium calculation is an important first step towards finding an appropriate process window for the BOF process and can be used as a guide for a subsequent full kinetic simulation. An example showing how to set up a kinetic simulation of the BOF process can be found in Thermo-Calc by navigating to the Help Menu → Example Files... → Process Metallurgy → PMET_04_Basic_Oxygen_Furnace_with_Kinetics.tcu. Read more about the example on our [webpage](#).