

**Application Example:**

# Using the Process Metallurgy Module to Calculate the Basic Oxygen Furnace (BOF) Process: with KINETICS

Database(s):	TCOX11 or newer, OXDEMO	Module(s):	Process Metallurgy Module
Version required:	Thermo-Calc 2021b or newer	Calculator(s):	Process simulation
Material/Application:	Steelmaking / Basic oxygen furnace		
Calculation name:	PMET_04_Basic_Oxygen_Furnace_with_Kinetics		

## INTRODUCTION

Thermo-Calc Software offers two application examples showing how the Process Metallurgy Module can be used to calculate the Basic Oxygen Furnace (BOF) process. This example simulates the kinetics of the BOF process, whereas the other only considers equilibrium. The kinetic model was introduced into the Process Metallurgy Module in Thermo-Calc 2020b. However, this example requires Thermo-Calc 2021b or newer. Or you can run a simplified version using the free Educational Package.

## How to Run the Calculation

This example includes three calculation files. They describe the same basic process, but one can be run with the free Educational version of the software, and they each use different elements. For the other two calculation files, you will need a license for Thermo-Calc 2021b or newer, and for one of them you will also need a license for the database TCOX11 or newer. In any case, you can read the PDF, which discusses the materials challenges and how Thermo-Calc can be used to solve them.

To run this example, open Thermo-Calc and navigate to the Help Menu → Example Files... → Process Metallurgy.

- **PMET\_04a\_Basic\_Oxygen\_Furnace\_Kinetics:** works with the free Educational Package and the OXDEMO database.
- **PMET\_04b\_Basic\_Oxygen\_Furnace\_Kinetics:** can be run with the OXDEMO database but requires a full license for Thermo-Calc 2021b or newer.
- **PMET\_04c\_Basic\_Oxygen\_Furnace\_Kinetics:** requires a full license for Thermo-Calc 2021b or newer and a license for the Metal Oxide Solutions Database TCOX11 or newer. This simulation corresponds pretty much to a real BOF process with the elements Fe, Mn, C, O, Ca, Al, Mg, Si, S, and P considered.

This example sets up a kinetic simulation of the BOF process shown in Figure 1 applying the Effective Equilibrium Reaction Zone (EERZ) model as outlined in Figure 2. Screenshots only show the set-up

for the most realistic calculation example (**PMET\_04c\_Basic\_Oxygen\_Furnace\_Kinetics**). The other examples are the same except that the elements that are not present in the databases are deleted.



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 carbon-rich hot metal (typical carbon content is about 4 - 4.5 wt%) coming from a blast furnace. The oxygen combines with the dissolved carbon to form CO and CO<sub>2</sub>, which escapes as a gas phase. The hot metal is thereby transformed into liquid steel with low carbon content ready for further refinement, casting and then rolling or forging. The basic process steps of the BOF process are displayed in [Figure 1](#) and listed directly below:

- 1) A scrap box containing a specific blend of scrap is charged into the BOF.
- 2) Hot metal, either coming directly from the blast furnace (BF) or from the hot metal desulfurization station, is poured into the BOF on top of the scrap.
- 3) The BOF is rotated into the upright position, the oxygen lance is lowered into the furnace and the blowing process starts.
- 4) Lance height and oxygen flow is varied during the blow, and fluxes or slag formers (mainly CaO and MgO) are added.
- 5) At the end of the process, the steel is sampled and corrective action taken if the specification is not met. It is then teemed into a ladle and sent to the ladle furnace or vacuum degasser where further steel refining processes are carried out.
- 6) The BOF slag is dumped into a slag pot and typically recycled in the blast furnace to recover the iron in the slag.

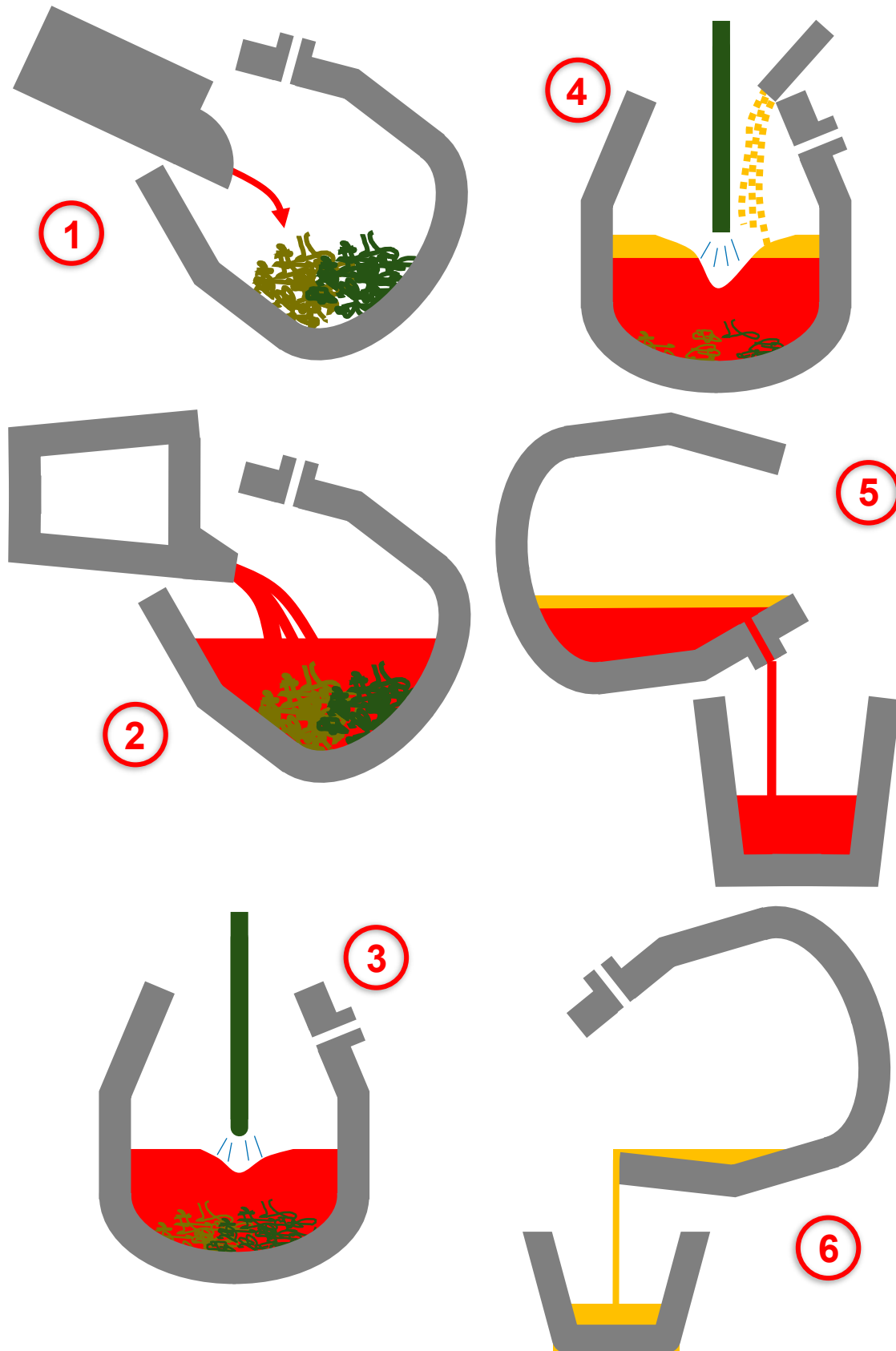


Figure 1. Basic steps of steelmaking in a basic oxygen furnace (BOF), as explained in the text.

## Kinetic Model for Describing Metallurgical Processes

Metallurgical processes such as this one rarely reaches equilibrium. Therefore, a model description must include kinetics if meaningful results are to be obtained. In recent years, a simple but powerful model termed *Effective Equilibrium Reaction Zone* (EERZ) has been developed and widely applied to simulate various metallurgical processes. The model was introduced into Thermo-Calc's Process Metallurgy Module beginning with the 2020b release. The kinetic process simulation in Thermo-Calc's Process Metallurgy Module is based on this model (see also Figure 2):

- 1) Initial situation with a liquid steel (steel zone) and slag phase (slag zone) next to each other, but *not* in equilibrium.
- 2) An EERZ is defined, encompassing a fraction of the liquid steel phase and a fraction of the slag phase. This fraction of the whole system is assumed to reach equilibrium during a given time step. The size of the zone determines the kinetics. A large EERZ results in fast kinetics, a small EERZ in slow kinetics. The factor defining the size of the EERZ is thus mass transport to and from the reaction zone.
- 3) The bulk chemical composition within the EERZ is calculated.
- 4) Equilibrium phase fractions, phase compositions and temperature within the EERZ is calculated.
- 5) The equilibrium oxide phases in the EERZ are mixed with the rest of the slag phase, and the metallic phases in the EERZ are mixed with the rest of the liquid steel.
- 6) A new liquid steel and slag composition is achieved that is closer to equilibrium. In the next timestep, the cycle restarts at 1.

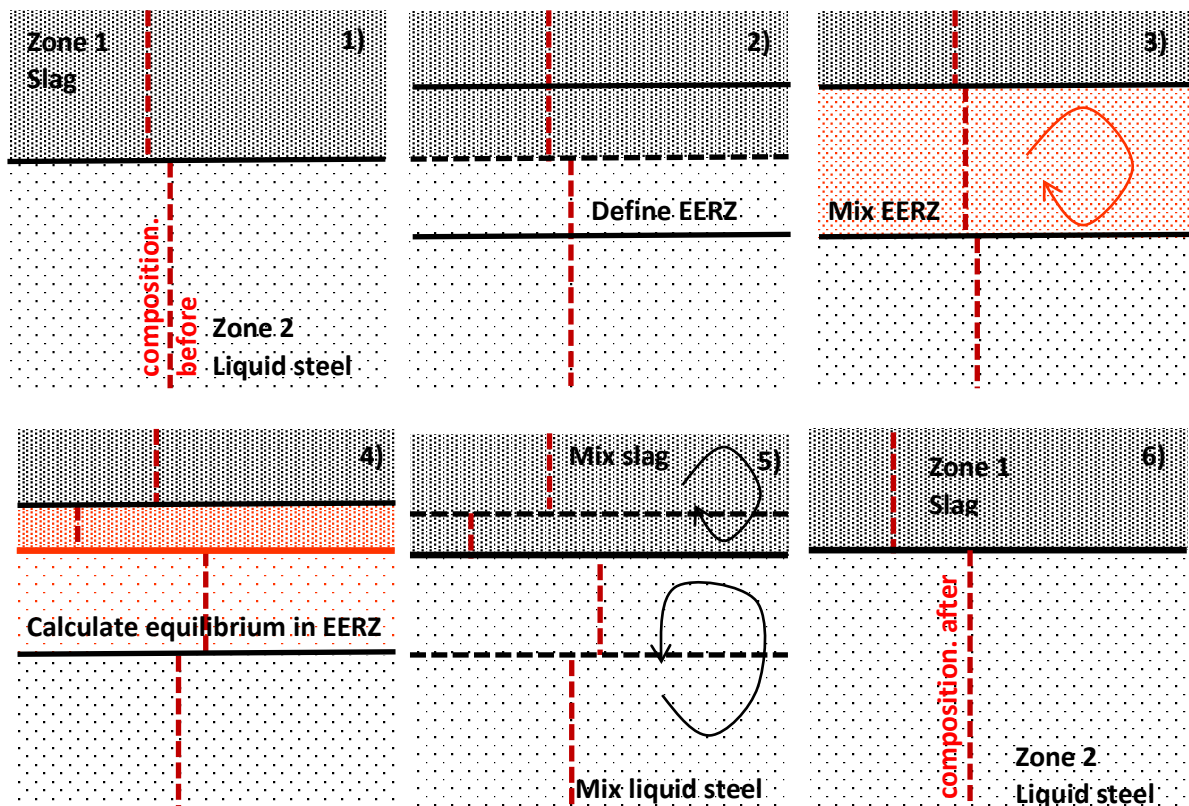


Figure 2. General principle of the Effective Equilibrium Reaction Zone (EERZ) model, which introduces kinetics to the simulation of the metallurgical process.

## EXAMPLE SET-UP: BASIC OXYGEN FURNACE KINETICS

### Three Steps to Set Up a Kinetic Simulation

A kinetic simulation in the Process Metallurgy Module requires setting up the following three steps, which are shown in Figure 3:

#### 1) Edit Process Model

In the first step, general kinetic parameters are defined in the Process Model. It is assumed that they are specific for the general process and the equipment size and shape that is used in the experiment and must only be defined once.

#### 2) Define Materials

In this step, all the material compositions that are to be used during the process are defined in the Materials tab.

#### 3) Define the Process Schedule

In this step, the steelmaking recipe is entered, which defines at what times how much of which materials are added to the BOF.

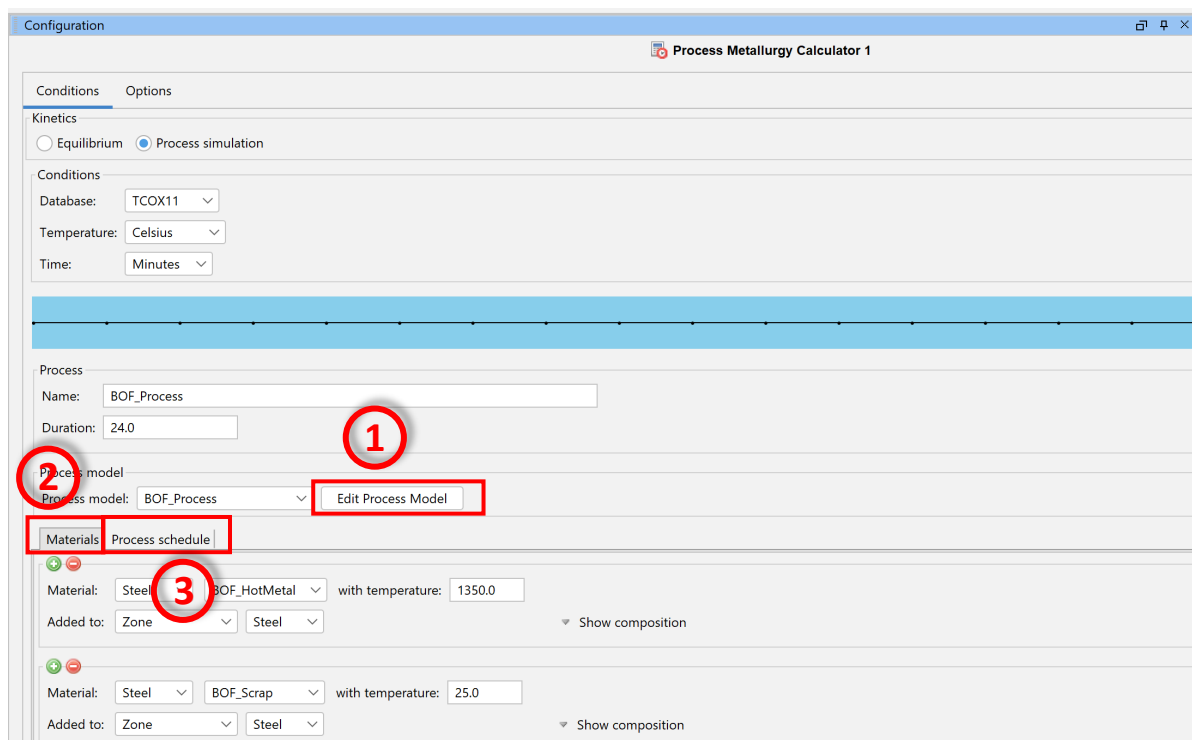


Figure 3. The three steps for settings up a kinetic simulation in the Process Metallurgy Module.

### Step 1: Edit Process Model

In the first step of the set-up, shown in Figure 4, various kinetic parameters are defined that are assumed to be related only to the type of process and geometry of the equipment used. The idea is that there is one set of parameters for the BOF, a different set of parameters for the ladle furnace, then different parameters for the vacuum degasser, and so on. The parameters should be left

unchanged for different chemical compositions and process parameters. The parameters to be defined on the **Edit Process Model** window are:

### 1) Pressure

Pressure can be either assumed to be constant or it can be changed in function of time. If it should change in function of time, then select **Table input** and enter the pressure in the process schedule table. Changing pressure is used mainly for processes that involve vacuum, like Vacuum Degassing (VD), Vacuum Oxygen Decarburization (VOD), Ruhrstahl-Heraeus Process (RH-Degassing), etc. Note that the pressure only influences reactions involving the gas phase.

### 2) Zones

Here the zones, as shown in Figure 2, are defined and can be given meaningful names. Note that in the current release, only two zones can be used. The zones must be assigned a fixed density<sup>1</sup>. When the checkbox **Allow degassing** is selected, any gas phase that forms during the process is removed at each calculation step and is not allowed to react with the zone. This type of calculation could be termed “open calculation”. It should be noted that the expansion work ( $P \cdot dV$ ) is always accounted for in the energy balance.

### 3) Reactions

This is where the kinetics of the reaction between the two zones is defined. The kinetics are a function of the area where reactions can take place (in this case the area of the steel-slag interface) and how fast the mass transport is to and away from this reacting interface.

In this example, the final amount of tapped steel should be ~100 t, having a volume of ~12 m<sup>3</sup>. Assuming the BOF is roughly cylindrical in shape and the depth of the liquid steel is ~2 m, we get a steel surface area (or slag-steel interface area) of 6 m<sup>2</sup>. Of course, in reality, there will be a large volume of a foamy steel-slag emulsion with a complex steel-slag interface and there might be more reaction zones that could be taken into account each having their own reaction kinetics. This is currently not possible with the Process Metallurgy Module. But in spite of this simplification, a very reasonable description of the BOF process can be achieved, indicating that the main processes are properly accounted for.

The reaction kinetics are defined by mass transfer coefficients in the steel and the slag. Many suggestions for numerical values can be found in the literature coming from experiments and CFD simulations. The values vary dramatically depending on how turbulent or agitated a process is. A good way of getting a feel for the kinetics is to calculate what fraction of steel and fraction of slag enters the EERZ per time. Here the mass transfer coefficient in the steel zone is 0.003 m/s or ~20 cm/min. As the height of the liquid metal is 2 m, this corresponds to approximately 10 % of the metal entering the EERZ and reacting with the slag per minute. The reaction rate of the slag is assumed to be 3 x slower due its higher viscosity. Again, the kinetic parameters can either be constant or change in function of time. If they should change in function of time, then select **Table input** and enter the pressure in the **Process schedule** table.

Transfer of phase group is primarily used to calculate inclusion flotation. For example, if a deoxidation agent such as Al is added to the liquid steel zone, solid Al<sub>2</sub>O<sub>3</sub> oxides (Corundum) might form. These gradually float up, out of the liquid steel and combine with the slag phase on top. The

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<sup>1</sup> Note that the density could be accurately calculated by Thermo-Calc as a function of composition and temperature. But in the Process Metallurgy Module, the density is only used to calculate approximate volumes that are in turn used to calculation the kinetic parameters, so an accurate value is not required. Calculating the density only unnecessarily increases calculation times.

settings shown in Figure 4 mean that 5 % of oxides are removed from the steel zone and transferred to the slag zone per minute.

#### 4) Heat

Here addition and removal of heat and heat transfer between zones is defined: The heat lost by convection and radiation is given as a constant value. For the heat that is added by active heating, for example using an electric arc, only the heating efficiency is given here<sup>2</sup>. The electrical power (in MW) and power-on, power-off times are given in the **Process schedule**.

As heat can be added to (or generated by exothermal reactions in) different zones, the temperatures of the steel zone, slag zone, and reaction zone can be very different. The parameter for the heat transfer coefficient controls how much heat flows from one zone to the other. A large value results in a quick equalization of the temperature.

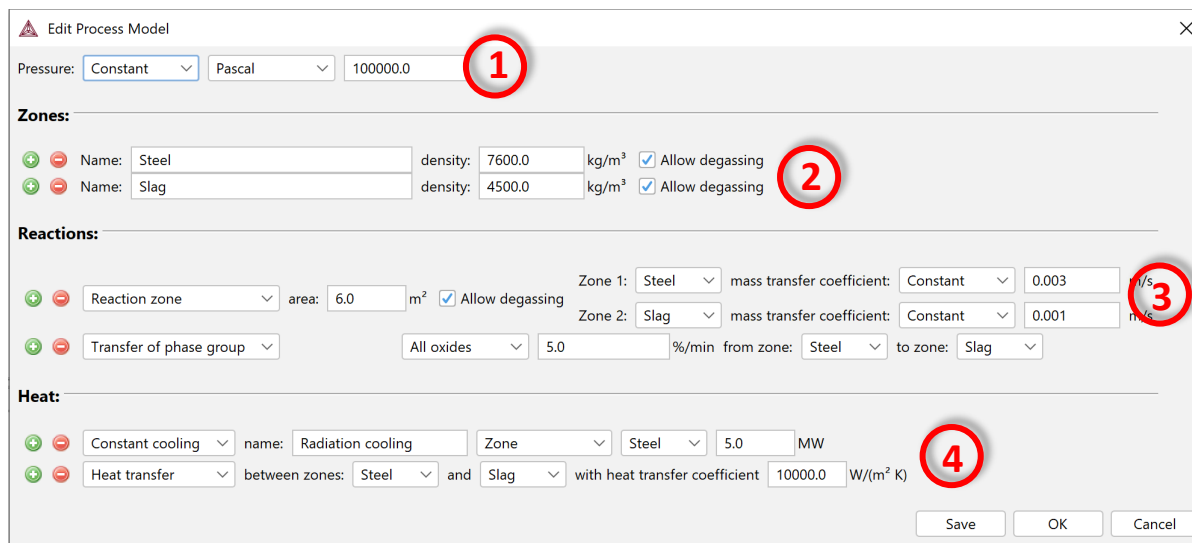
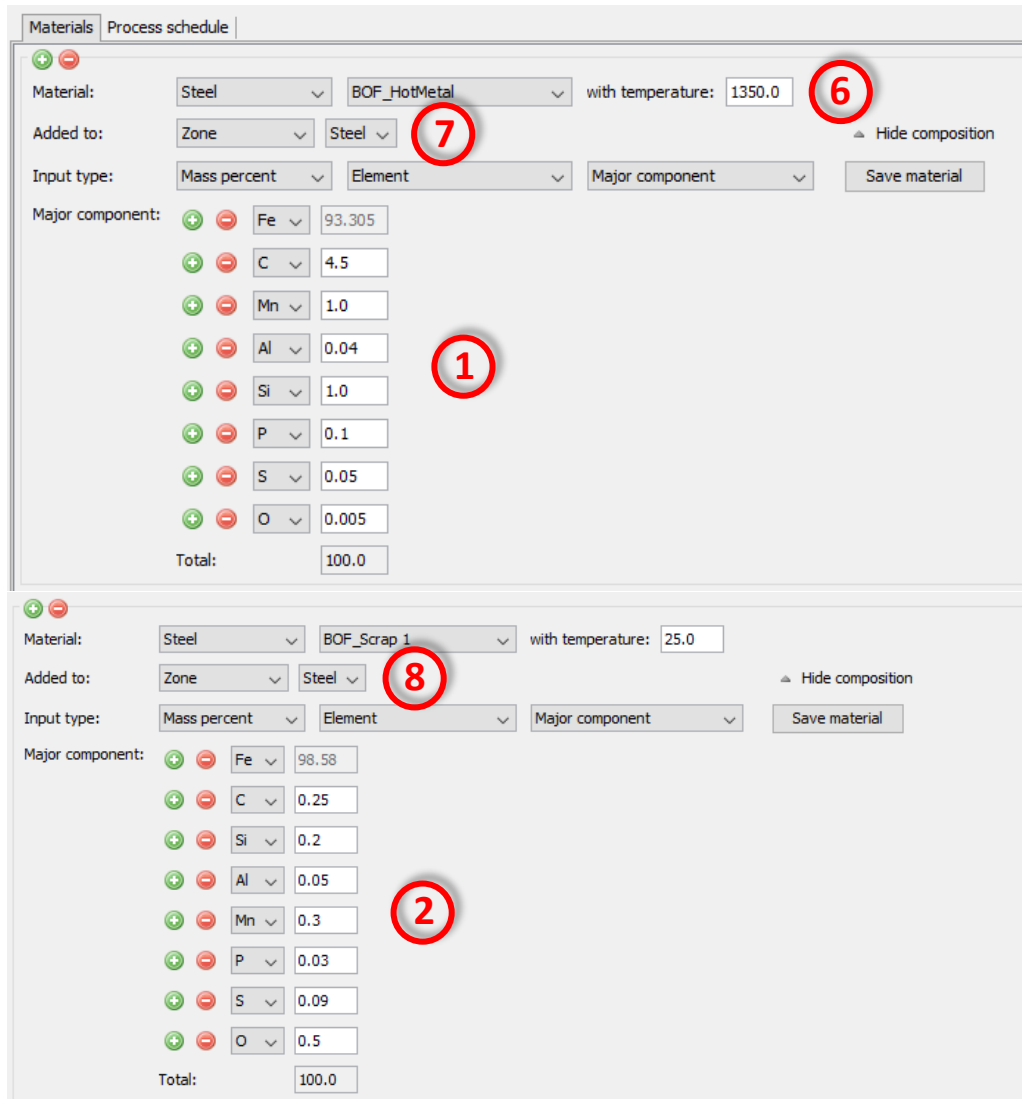


Figure 4. Basic settings for kinetic simulations in the Process Metallurgy Module. These settings are related to the type of process being simulated and the geometry of the equipment being used. Therefore, they should only have to be set up once for a given piece of equipment.

<sup>2</sup> The reason for this is that usually the electric power is known (for example 15 MW for a typical ladle furnace or 80 MW for an electric arc furnace). How much of this energy actually enters the steel as heat is given by the efficiency, which might be around 60 - 80 %.

## Step 2: Define Materials / Chemical Composition

All the chemical compositions of the raw materials that are going to be used can be defined and stored in the software for repeated use, the idea being that users can compile a library of materials regularly used in their own steel plant or research facility. This allows one to pick and choose materials instead of having to re-enter them for each calculation. The compositions of the material used in this simulation are shown in Figure 5, with an explanation following the image.



The screenshot shows the 'Materials' tab in the Thermo-Calc software. It displays two material definition panels. Red circles 1 through 8 highlight specific fields and buttons:

- Circle 1:** Points to the 'Major component' list for 'BOF\_HotMetal'.
- Circle 2:** Points to the 'Major component' list for 'BOF\_Scrap 1'.
- Circle 3:** Points to the 'Fe' input field for 'BOF\_HotMetal'.
- Circle 4:** Points to the 'Fe' input field for 'BOF\_Scrap 1'.
- Circle 5:** Points to the 'C' input field for 'BOF\_HotMetal'.
- Circle 6:** Points to the 'with temperature' field for 'BOF\_HotMetal'.
- Circle 7:** Points to the 'Added to' dropdown for 'BOF\_HotMetal'.
- Circle 8:** Points to the 'Added to' dropdown for 'BOF\_Scrap 1'.

**Material: BOF\_HotMetal** (with temperature: 1350.0)

Added to: Zone Steel

Input type: Mass percent Element Major component Save material

Major component:

Element	Value
Fe	93.305
C	4.5
Mn	1.0
Al	0.04
Si	1.0
P	0.1
S	0.05
O	0.005
<b>Total:</b>	<b>100.0</b>

**Material: BOF\_Scrap 1** (with temperature: 25.0)

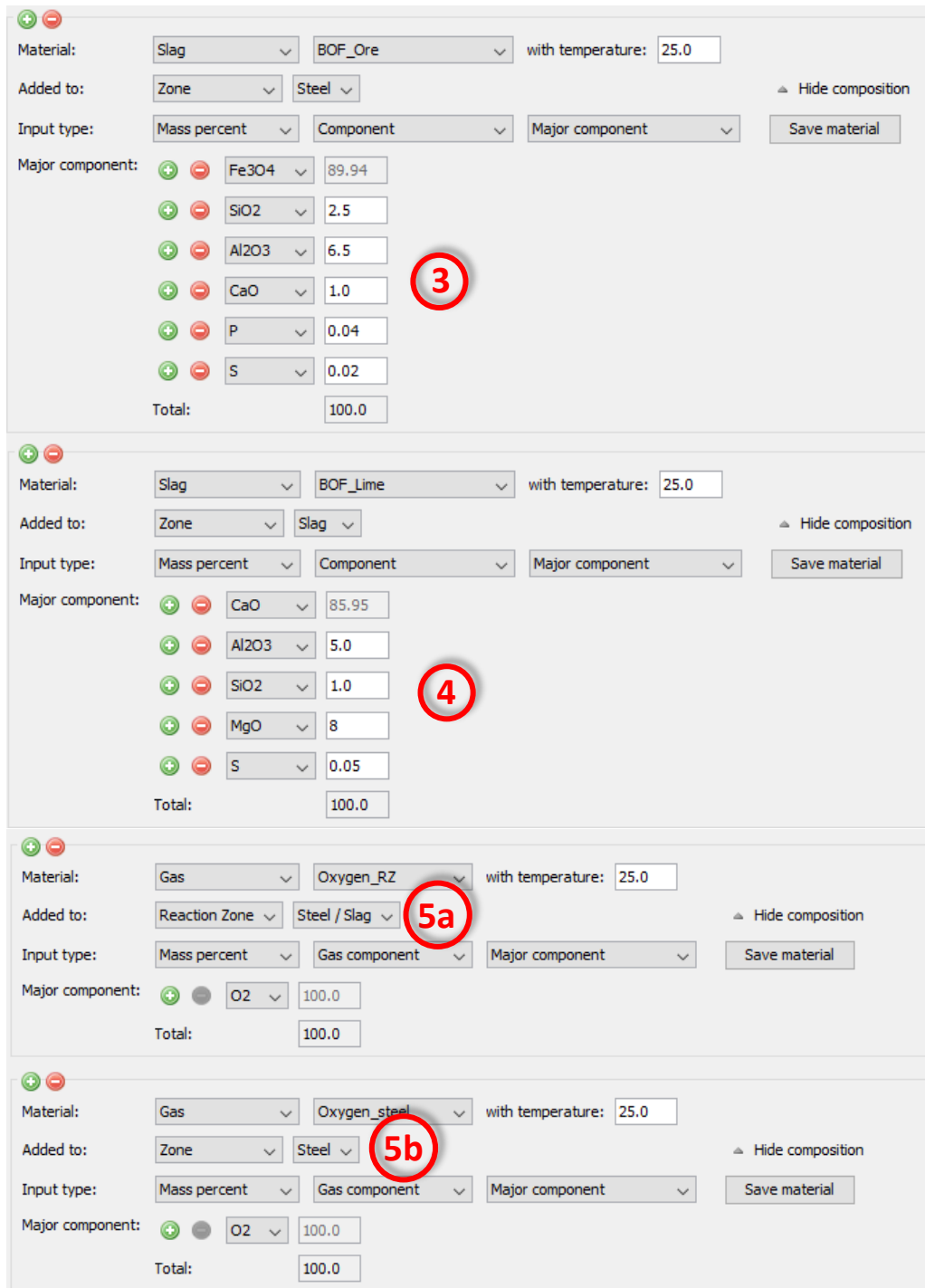
Added to: Zone Steel

Input type: Mass percent Element Major component Save material

Major component:

Element	Value
Fe	98.58
C	0.25
Si	0.2
Al	0.05
Mn	0.3
P	0.03
S	0.09
O	0.5
<b>Total:</b>	<b>100.0</b>





The screenshot displays four panels for defining materials in the software. Each panel has a consistent layout with the following fields:

- Material:** A dropdown menu.
- Added to:** A dropdown menu.
- Input type:** A dropdown menu.
- Major component:** A list of components with checkboxes and input fields for mass percent.
- Total:** A text box showing the sum of components.
- Buttons:** 'Save material' and 'Hide composition'.

Red circles with numbers highlight specific inputs:

- 3:** Points to the 'CaO' component input field in the first panel (BOF\_Ore).
- 4:** Points to the 'MgO' component input field in the second panel (BOF\_Lime).
- 5a:** Points to the 'Oxygen\_RZ' material dropdown in the third panel.
- 5b:** Points to the 'Oxygen\_steel' material dropdown in the fourth panel.

Material	Added to	Input type	Major Component	Mass Percent	Total
Slag	Steel	Mass percent	Fe3O4	89.94	100.0
			SiO2	2.5	
			Al2O3	6.5	
			CaO	1.0	
			P	0.04	
			S	0.02	
Slag	Slag	Mass percent	CaO	85.95	100.0
			Al2O3	5.0	
			SiO2	1.0	
			MgO	8	
			S	0.05	
Gas	Reaction Zone	Mass percent	O2	100.0	100.0
Gas	Steel / Slag	Mass percent	O2	100.0	100.0

Figure 5. A screenshot of the software showing the compositions and input temperatures of the materials that are to be used in the process and which zone they are to be added to.

The compositions are somewhat simplified compared to a real industrial case with minor elements and tramp elements not included. It is generally a good strategy to simplify the simulation as much as possible, as the first aim must be to get the model running and giving reasonable results. Complexity can be added later.

## Comments on the Selected Compositions of Input Materials

### 1) Hot metal

Carbon: Hot metal coming from a blast furnace usually has a C content of 4 to 4.5 wt%, which is the amount in equilibrium with graphite in the hot zone of the blast furnace (typically 1320 to 1370 °C). This means that the C content of the hot metal can be read off the Fe-C phase diagram. High temperatures in the blast furnace results in higher content; lower temperatures result in lower C content. This relationship is accurately known, meaning that measuring the temperature is enough to deduce the C content of the hot metal.

- Silicon: The Si content can vary between 0.3 and 1.5 wt%. The exothermic oxidation of Si is an important heat source in the BOF. High Si contents, therefore, require more cooling scrap or cooling iron ore to be added. High Si contents also result in the formation of more and more acidic slag.
- Phosphorous and sulfur: For this example, the S content is high at 0.05 wt%. This would be typical if no hot-metal desulfurization was carried out. Also, the P content is high at 0.1 wt%. This is a typical value obtained if the BOF slag is recycled in the BF.

### 2) Scrap

A typical scrap composition is used here. In reality a blend of different types of scrap would be added to the scrap box. Also, certain ferroalloys might be added such as Ni or Mo. These are not easily oxidized, so they remain in the liquid steel. Other elements such as Cr or Mn are more easily oxidized, so adding these elements to the BOF is not a good idea as it would simply result in them being oxidized and moved to the slag phase. Cu is also an element that is not easily oxidized, meaning that it cannot be effectively removed in the BOF and will remain in the liquid steel. In most steels, Cu is unwanted. The only way of lowering the Cu content is by careful selection of scrap material (a major source of contamination by Cu) and dilution with raw materials that have a low Cu content.

Scrap is always partially corroded and may contain humidity. Standard practice is to assume a fully metallic scrap composition and correcting the amount added by a yield factor. This is not good practice because to obtain correct mass and energy balance, *all* the material entering the furnace must be accounted for. Increasing the oxygen content and possibly also hydrogen content to account for humidity and hydroxides/rust is a better and more realistic approach as this way not only is the mass balance correct, but also the increased cooling effect of corroded scrap is considered. In this example we ignore H, but increase the oxygen content somewhat.

### 3) Ore

Iron ore is added as the iron source and also for cooling the hot metal. Oxide materials, as well as carbonates such as limestone ( $\text{CaCO}_3$ ), are effective coolants due to the endothermic decomposition reactions taking place. Ore must be added early in the process when the oxygen activity in the hot metal is still low, allowing the ore to be reduced and dissolved in the hot metal. Many other additions are made to the BOF: waste oxides from other areas of the steel plant, such as mill scale, are added to recycle them, direct reduced iron (DRI) is added as a coolant and/or source of iron, and so on. Each of these additions comes with its own set of process challenges. The Process Metallurgy Module is an efficient way of investigating and understanding the fundamental thermodynamic aspects of such additions.

### 4) Slag formers

High CaO slag formers are added mainly to remove the unwanted P from the hot metal. The oxide liquid (slag) that is formed is aggressive towards the refractory lining of the BOF and can lead to slag-

line erosion. The refractory used in a BOF is high in MgO (a “basic” oxide, thus the name basic oxygen furnace). To protect the refractory, the slag is usually enriched with MgO. If the slag is saturated in MgO (or in other words, the MgO content in the liquid oxide is close to the solid MgO + Oxide liquid equilibrium), then far less of the refractory material is dissolved by the slag.

### 5) Oxygen

In this example, the blown oxygen is pure O<sub>2</sub>. In reality it contains traces of Ar or N<sub>2</sub> that dissolve in the liquid steel and slag. Especially N can result in problems during later processing. The solubility of N in liquid steel and slag is included in the database, so the effects of N or other impurities can be investigated if desired.

### 6) Temperature of added materials

Because the calculations are performed under adiabatic conditions, the temperature of each of the additions must be specified. The global temperature is then calculated considering any exothermic or endothermic reactions that might occur.

### 7) Zone to which the materials are added

The zone to which a material is added has a profound influence on the result of the simulation.

Figure 6 illustrates how the selections made in the Process Metallurgy Module relate to the process in the BOF. Oxide materials that are added tend to float on the hot metal and be dissolved in the slag, thereby changing its composition. This means that adding them to the slag zone is the most reasonable choice. Metallic additions tend to sink through the slag and down through the liquid hot metal, and the most reasonable choice is to add them to the steel zone. It is also possible to add materials to the reaction zone (or EERZ). This often makes sense for materials that are injected, such as oxygen in this example, but this could also be lime or carbon powder.

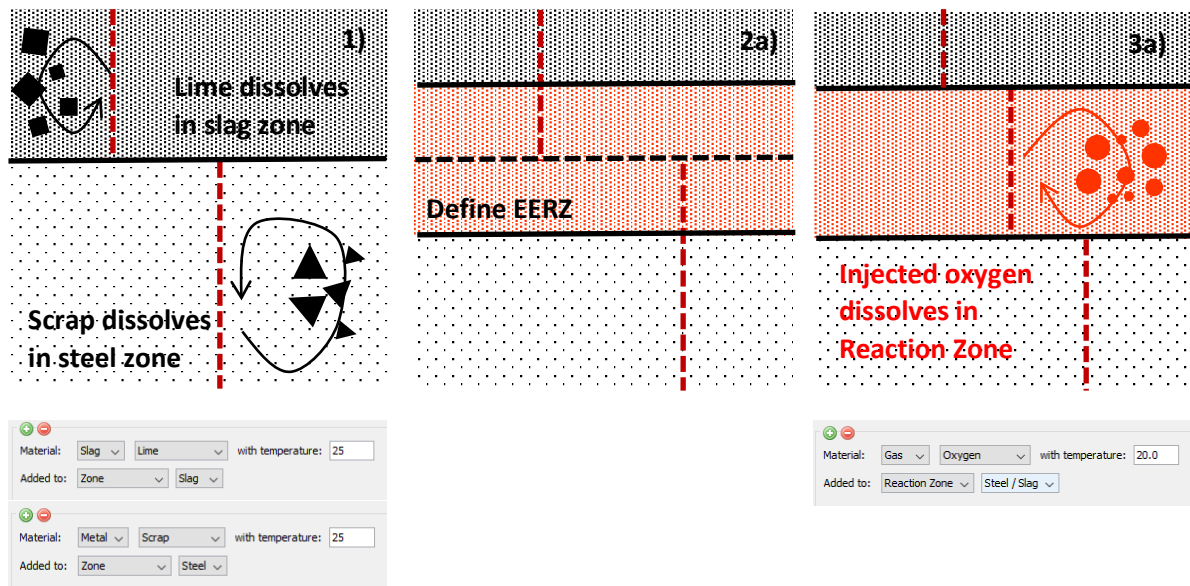


Figure 6. Illustration showing the meaning of which zone the material are added to and screenshots showing how to define it in the Process Metallurgy Module.

The injection of oxygen is used to illustrate the importance of selecting the correct zone to which a material is added. If we choose to add the oxygen to the slag zone, nothing much happens; the oxygen does not react with the oxide slag and leaves the system as relatively pure oxygen exhaust

gas. This is not a good choice. If the oxygen is added entirely to the steel zone, then it is considered to react with all the 100 t of hot metal. The elements in the hot metal quickly oxidize, C forms CO / CO<sub>2</sub> gas and other easily oxidized elements in the hot metal form oxides (solid or liquid) inside the steel zone. A small part of these oxides is transferred to the slag phase per time-step according to the parameter set for **Transfer of phase group** on the **Edit Process Model** window. Another part mixes with the slag in the reaction zone. If the oxygen is added entirely to the reaction zone, then it is possible that the reaction zone is completely oxidized. This is probably also not a good representation of the real process because what should happen is that an equilibrium is reached between liquid metal in contact with the liquid slag.

There are two ways of preventing such a complete oxidation of the reaction zone. First it must be assured that the reaction zone is adequately big (so high values of mass transfer) so it cannot be fully oxidized, and second, one can split the oxygen addition, adding one part to the steel zone and another part to the reaction zone. The part of the oxygen added to the steel zone is assumed to penetrate deep into the hot metal, forming oxides that essentially remain in the liquid steel as inclusions. This is what has been done in this example.

### 8) Adding “foreign” materials to a zone

It is also possible to add non-metallic materials to the steel zone and metallic materials to the slag zone. The addition of iron ore (which is an oxide) to the steel zone for example. This can result in the steel zone having oxide inclusions or the slag zone having metallic inclusions. Such “foreign” materials can also form in-situ through chemical reactions. The best-known example of this is the formation of oxide inclusions by adding a deoxidizing agent (typically Al or SiMn) to a liquid metal with a high amount of dissolved oxygen. Correspondingly, slag conditioners such as Al or CaC<sub>2</sub> can be added to the slag where they reduce FeO in the slag to metallic Fe. The movement of such foreign phases (inclusions) from one zone to the other is controlled by the **Transfer of phase group** setting found on the **Edit Process Model** window.

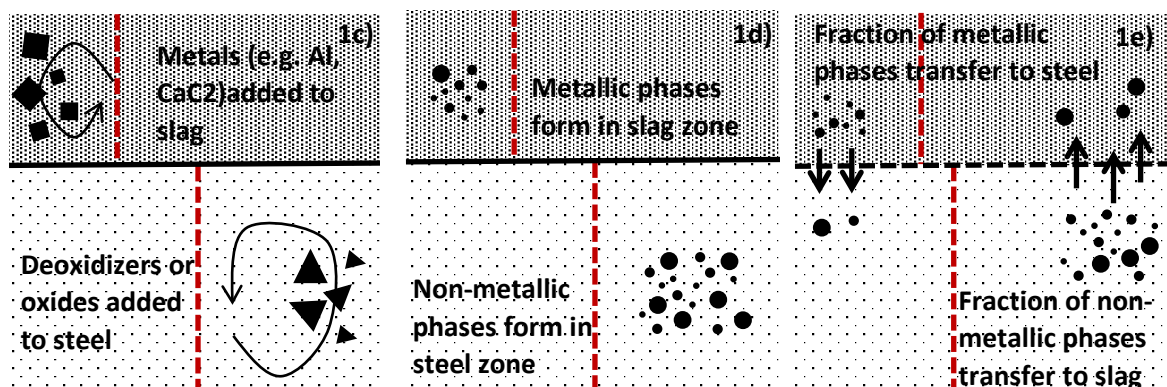


Figure 7. Illustrations showing the formation of “foreign” phases withing a zone.

Despite the model being seemingly simple, there is a lot of flexibility to consider as all sorts of processes might be occurring.

### Step 3: Define the Process Schedule

The third and last step in setting up a kinetic simulation is to set up the Process Schedule. This is the actual steelmaking recipe that defines at which time how much of which material is added to the BOF. The total amounts of material added in this example are based on the very rough estimation of the amounts of material required to produce 100 t of liquid steel shown in Table 1.

*Table 1. Approximate amounts of raw materials required to produce 100 t of liquid steel in a BOF.*

<u>Input</u>		<u>Output</u>	
Hot metal:	87 t	<b>Liquid steel:</b>	<b>100 t</b>
Scrap:	22 t	Slag:	13 t
Lime (CaO)	5 t	Exhaust gas (CO / CO <sub>2</sub> )	10 t
Ore	2 t	Fumes / dust	1 t
Oxygen	8 t (6000 Nm <sup>3</sup> )		
Total	124 t	Total	124 t

In practice, scrap is charged into the BOF first by tipping the scrap box. Hot metal is subsequently poured on top of the scrap, and slag formers (mainly burnt lime and dolomite) are added through a chute in the early stage of oxygen blowing. It takes some time for the scrap and slag formers to be heated to the same temperature as the hot metal, to melt and dissolve. This is accounted for in this example by adding it with a feeding rate of 2000 kg / min for a total of 11 min. This corresponds to the assumption that the 22 t of scrap that is added to the converter melts at a constant rate and is fully dissolved in the hot metal after 11 minutes. An alternative approach would be to make several one-time additions. Adding all 22 t at time 0 is probably not a good approximation, as this would result in the scrap equilibrating with the hot metal in one single timestep. This is not what happens in reality. In the near future, the possibility to add a third zone for the reaction of the solid scrap with the liquid hot metal, or alternatively a melting model represented by a power-law or Arrhenius equation might be implemented in the Process Metallurgy Module. However, neither of these approaches are currently available.

The process schedule for this example is shown in Figure 8.

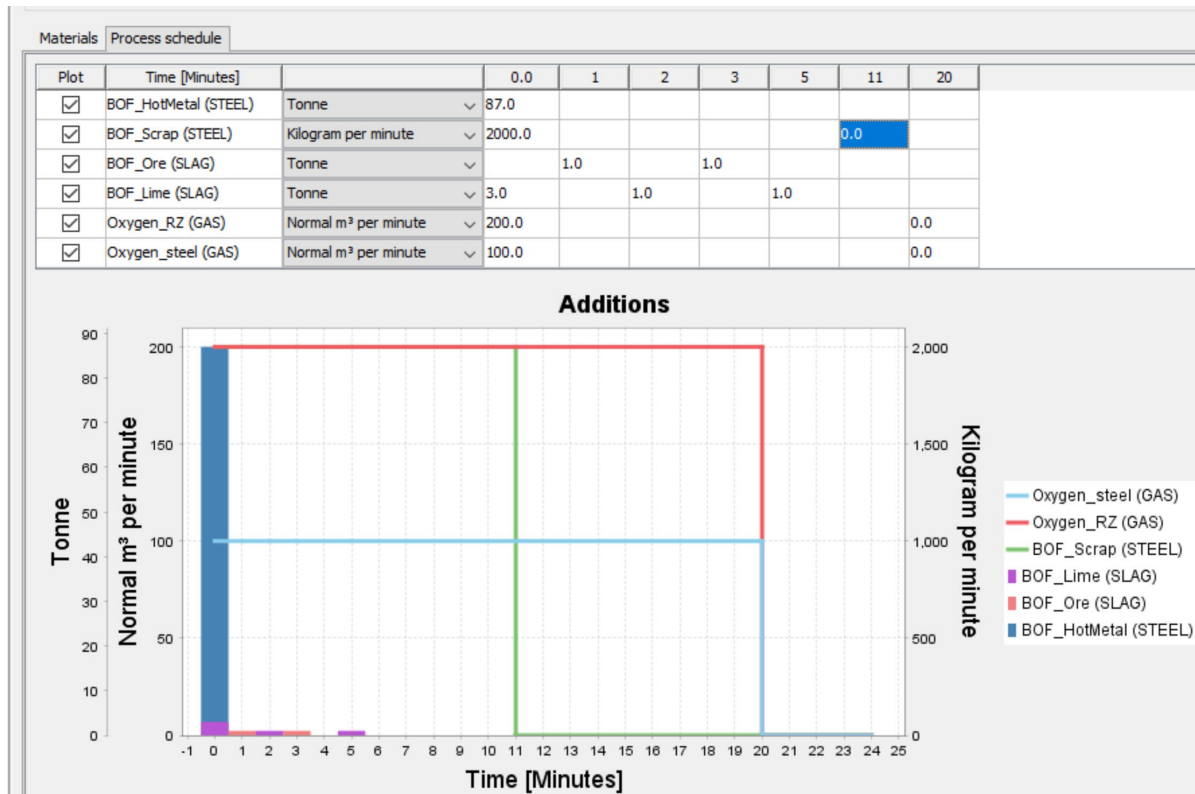


Figure 8. Process schedule for the production of approximately 100 t of steel in a BOF. Note that the gradual melting of the scrap at the bottom of the converter is simulated by assuming a constant addition of 2000 kg / min for a period of 11 min.

## EXAMPLE RESULTS

Many different aspects of the reactions taking place in the BOF can be plotted and analyzed. Only some are presented and discussed here.

### Temperature

The temperature increases in the BOF, as shown in Figure 1Figure 9, is due to the exothermic reaction of oxygen with the Si and C dissolved in the hot metal. However, this heat is not generated throughout the system equally, but within a rather small volume that actually comes into contact with the oxygen. In this example, most of the oxygen is added to the reaction zone, so this is where most heat is generated and thus the temperature is highest. Part of the oxygen is assumed to react with the steel zone, so this zone is also actively heated. The temperature is then equalized by the heat transfer between the zones as defined on the **Edit Process Model** window. It is interesting to note that the slag zone is hotter than the steel zone even though it is not actively heated by any exothermic reactions. The reason for this is simply that its mass is smaller than the mass of the steel zone, so it is heated up quicker by the hot reaction zone.

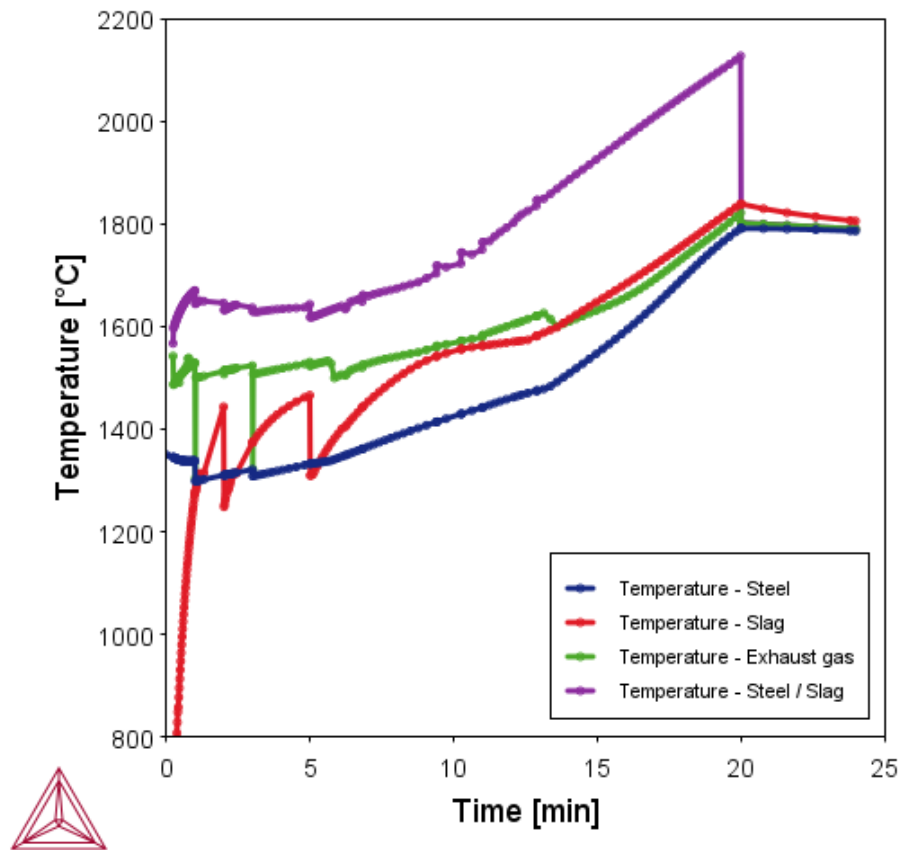


Figure 9. Temperature evolution of the steel zone (the bulk of the hot metal that is transformed into steel), the slag zone, the Steel / Slag reaction zone and the exhaust gas. Note that the temperature of the Steel / Slag reaction zone is highest as this is where most of the oxygen reacts. The heat that is generated here flows into the steel and slag zone according to the heat transfer coefficient defined in the Process Model, thereby increasing the temperature of the whole system.

## Liquid Metal Composition and Amount

The main purpose of the BOF is to convert the carbon-rich hot metal from the blast furnace to low carbon steel suitable for rolling and forging. However, other elements are also oxidized and transferred to the slag phase, thereby removing them from the liquid metal. Removing certain elements is highly desirable, such as the oxidation and removal of phosphorous by the following reaction:



Other oxidation reactions, such as the oxidation of Cr (not considered in this example) or Mn, are undesirable, as they result in the loss of these valuable elements to the slag phase. For many steel grades they must be alloyed back into the steel at a later stage using expensive ferroalloys. The changes in chemistry of the hot metal can be seen in Figure 10.



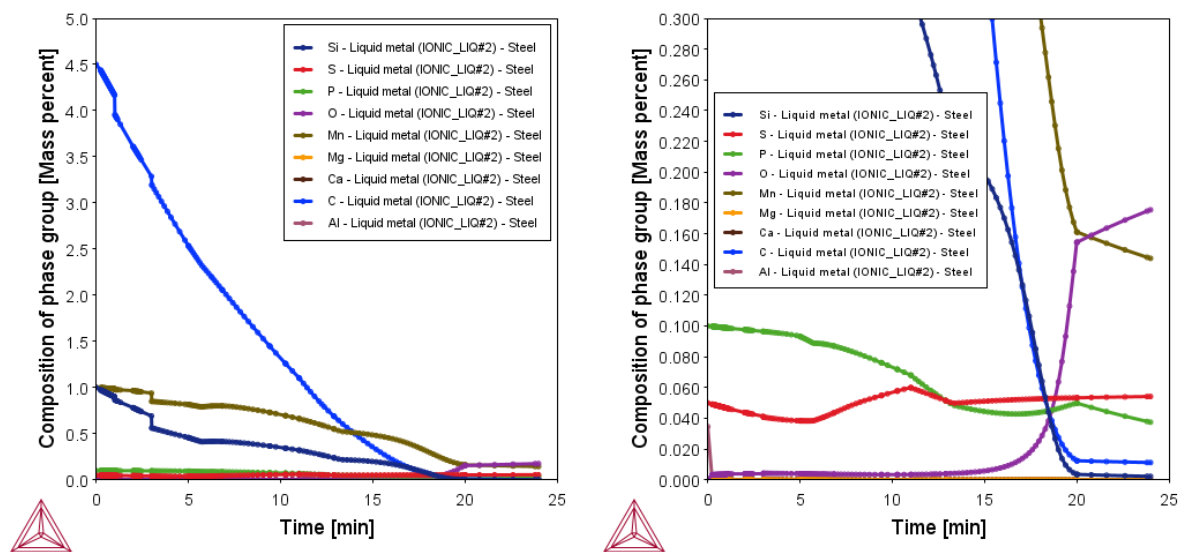


Figure 10. Evolution of the steel chemistry during oxygen blowing. Left and right plots have different scales. On the left the reduction of easily oxidized elements C, Si and also Mn is visible. On the right plot the removal of P can be seen. It can also be seen how, at the end of the oxygen blow, the dissolved oxygen in the steel increases sharply when there is no carbon left to oxidize. In this case, too much oxygen was blown into the steel. The blowing process should have been stopped about 2 minutes earlier.

Looking at the chemistry change at the very end of the blow (between 18 and 20 min), a dramatic increase of the dissolved oxygen in the liquid steel is observed (right plot, purple line). This happens because there is no carbon left in the steel to be oxidized. In reality the time at which this happens can be easily detected by the change of the flame appearance at the mouth of the BOF. If the blowing process is continued, the oxygen oxidizes iron resulting in a loss of yield, the temperature of the steel continues to increase and the large amount of dissolved oxygen needs to be removed by killing the steel when the furnace is tapped. These are severe problems that disrupt further processing downstream. Therefore, it is extremely important to avoid such an “over-blow”.

## Slag Composition and Amount

Copious amounts of slag are formed in the BOF during steelmaking. If low carbon contents are to be achieved, a high content of FeO in the slag is unavoidable. This is, of course, iron that is lost in the process, resulting in a lower yield. In most plants the converter slag is fed into the blast furnace to recover this iron. However, this also means that the P removed from the hot metal is returned back into the blast furnace, resulting in hot metal with a high P content that must again be removed in the BOF. Figure 11 shows the evolution of the slag amount and slag composition during the BOF process: the total amount of slag increases, and fraction of liquid slag also increases. Initially the slag becomes richer in SiO<sub>2</sub> as this is the first element that is oxidized (apart from carbon, which does not dissolve in the slag phase but escapes as CO / CO<sub>2</sub> gas). Later the MnO content in the slag starts increasing and after about 6 minutes, when the carbon content in the hot metal has dropped to about 2 wt%, the FeO content in the slag starts increasing. At the end of the process, the FeO content of the slag reaches > 40 wt%.



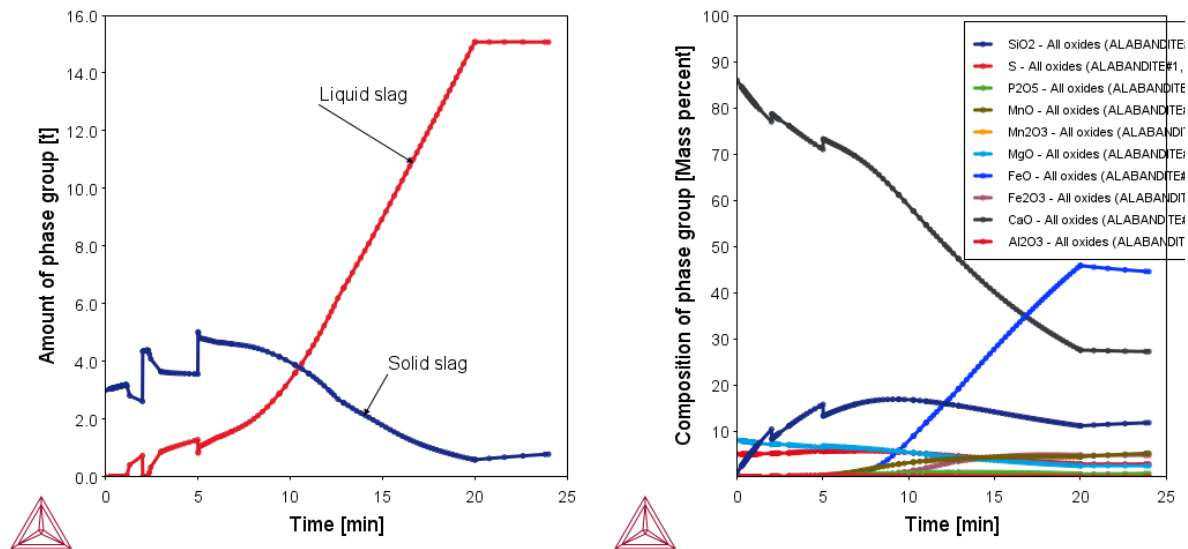


Figure 11. Amount (left) and composition (right) of slag formed during the BOF process.

## Exhaust Gas Composition and Amount

The way the gas that evolves during the process is accounted for is that it is removed from the reacting system at every time step. The amount, temperature, and composition of the exhaust gas is stored, but it does not participate in any further reaction. Figure 12 shows that the total amount of gas produced is about 9 t. While the exhaust gas contains traces of other elements, the main components are CO and CO<sub>2</sub>. According to the calculation, the composition of the exhaust gas is about 98.5 wt% CO and 1.5 wt% CO<sub>2</sub>. Measurements of the off-gas composition of a BOF show that in the real process the gas composition is closer to 90 wt% CO and 10 wt% CO<sub>2</sub>. The reason for this discrepancy is that part of the oxygen gas that is injected does not react in the reaction zone. This unreacted oxygen escapes and reacts with the CO in the exhaust forming CO<sub>2</sub>. In the 2020b release of the software, such post-combustion reactions are not possible to implement. The only way of considering this is by reducing the amount of gas injected by an oxygen yield factor. No such yield factor is introduced in this example. This explains why, despite using a typical amount of 6000 Nm<sup>3</sup> of O<sub>2</sub> gas per 100 t of hot metal, the calculation shows quite significant “over-blow” as discussed above and shown in Figure 10.

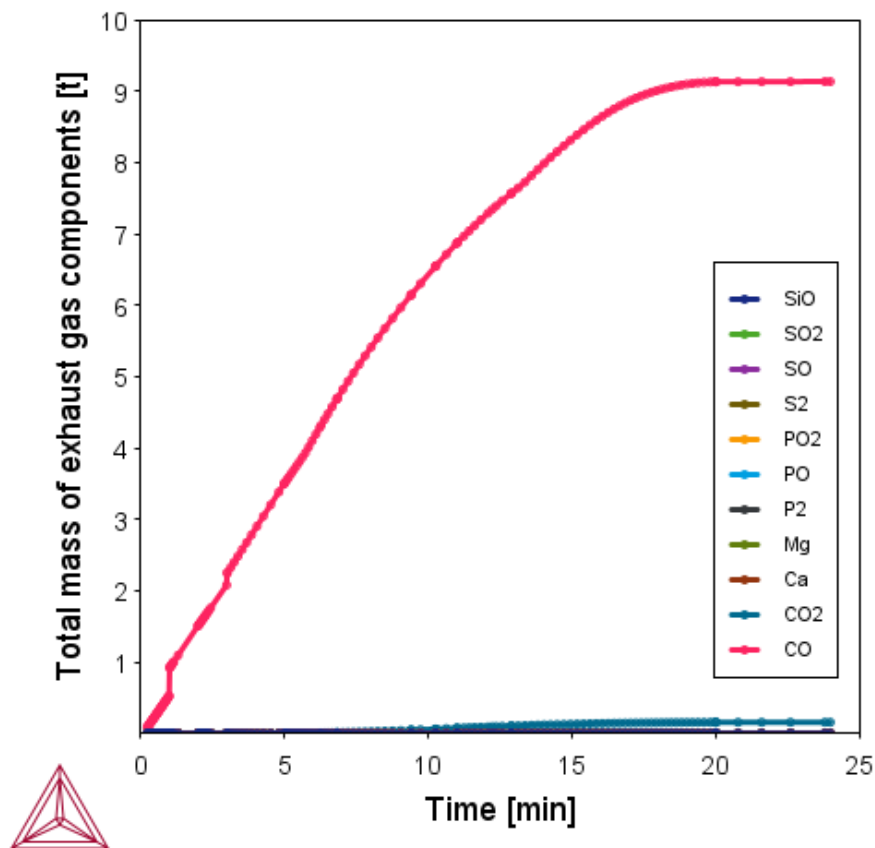


Figure 12. Amounts of gas components in the exhaust gas as a function of time.

## Parameters Used for the Simulation

Steelmaking in a BOF is a highly complex process. A good model description should capture all the important features with a minimum number of arbitrary or adjustable parameters. In the model presented here, several fundamental aspects are rigorously accounted for such as mass and heat balance. Additionally, the underlying fundamental thermodynamic equilibria such as the reaction between the liquid steel and the slag phase or the reaction of the oxygen gas with the hot metal are accounted for in a highly sophisticated manner through the use of the CALPHAD method and the powerful TCOX thermodynamic database.

The reaction kinetics, on the other hand, are accounted for using a strongly simplified model with rather arbitrary adjustable parameters that are defined on the **Edit Process Model** window. Other choices made when setting up the model are also, to some extent, arbitrary. In this case they include the step-wise addition of scrap and slag formers, which is supposed to simulate the fact that not all the scrap and slag formers that are added at the start of the project are immediately melted, but instead gradually heat up, melt, and dissolve in the hot metal or slag phase. Another choice is to decide where the blown oxygen reacts: either exclusively in the turbulent reaction zone where there is an emulsion of hot metal and slag, or whether part of the oxygen penetrates deep into the hot metal and oxidizes it without much interaction with the CaO - rich slag phase. In this example – in the absence of anything better – all these parameters are based on common sense choices and aim to qualitatively reproduce the basic processes known to occur in a BOF from textbooks. There are

several plots that can be consulted to help decide if the choices made really are reasonable. Two such examples are shown in Figure 13.

The plot on the left shows the amount of oxides formed in the steel zone. Most of these are formed due to the oxidation of components of the hot metal by the fraction of oxygen that is added to the steel zone (see note 5b in Figure 5). If the composition of these inclusions is plotted, it is found that, to start with, they are rich in  $\text{SiO}_2$ , which makes sense as the oxygen first oxidizes the Si dissolved in the hot metal. In a later stage they are rich in FeO, which again makes sense, as when there is neither abundant Si nor C in the hot metal, Fe starts to oxidize. The amount of these oxides in the steel zone decreases as a function of time due to the **Transfer of phase group** parameter set on the **Edit Process Model** window. The simulations suggest that at the end of the blowing process the steel zone contains about 1 t of FeO rich liquid inclusions. This sounds plausible and is important information for subsequent processing of the steel as the carryover of this FeO-rich oxide liquid into the ladle is unavoidable and has a big influence on subsequent steel refining. It changes the amount of Al or SiMn that needs to be added to deoxidize the steel on tapping and it results in a FeO contamination of the steel-refining slag that is added during ladle refining.

The plot on the right in Figure 13 shows the amount of each phase group in the reaction zone directly after the equilibrium calculation per calculation time-step. The amount of phase group in the reaction zone is a direct result of:

- 1) The kinetic parameters defined in the Process Model, in other words, the Mass transfer coefficient in the steel zone and in the slag zone (see number 3 in Figure 4). A larger number (faster mass transfer) results in a larger amount of phase groups in the reaction zone and vice versa.
- 2) The length of the calculation timestep: If the calculation timestep is small, the amount of the phase groups is small, for longer time-steps the amount is larger.

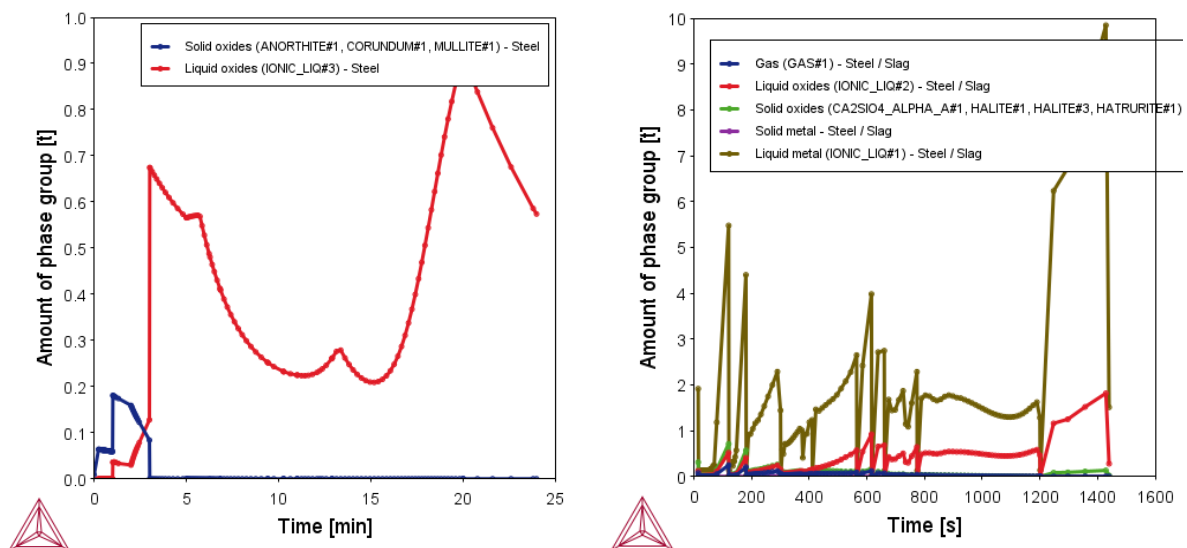


Figure 13. Evolution of oxide inclusions in steel zone (left) and size of steel / slag reaction zone per calculation time-step (right).

The Process Metallurgy Module dynamically adjusts the size of the calculation time-step to optimize numerical accuracy and improve calculation convergence. When material is added, the time-step is automatically decreased. This is the reason for the small amount of phase groups in the reaction

zone at the times when material is added. Checking the **Event log** in Thermo-Calc, it can be seen that between 15 min and 20 min, the time-step is approximately 12 s. From [Figure 13](#) it can be estimated that about 2 t of material reacts in the steel / slag reaction zone during these 12 s (about 1.7 t of liquid metal and about 0.3 t of liquid oxides (or slag)). This means that about 10 % of the total material reacts per minute, which accurately corresponds to the estimation based on the mass transfer coefficients outlined in the section describing the Process Model.

The important aspect of this figure is that it contains both liquid metal and liquid oxide. This shows that the amount of oxygen added to the reaction zone per time-step does not fully oxidize the metal. If the amount of liquid metal in the reaction zone is very small, then this indicates that all the liquid metal entering the reaction zone is oxidized and is thereby transferred to the slag zone. No equilibrium between the liquid metal and the slag is established and the simulation probably does not represent the reaction taking place in the real BOF very well.