

# Calculating Steel Making and Steel Refining Processes using Thermo-Calc's New Process Metallurgy Module and the CALPHAD Database TCOX9

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## Abstract

Computational thermodynamics is a powerful tool widely applied in materials science, e.g. for alloy design. Thermodynamic databases developed through the CALPHAD approach usually give reasonable predictions of thermodynamic properties as well as the phase equilibria of corresponding multi-component systems.

A thermodynamic database, TCOX, has been developed for calculating thermochemical interaction between liquid steel and slag. With the TCOX database an attempt is made to develop an internally consistent database for oxygen-containing systems. Today the TCOX database includes the major alloying elements in steels as well as the important slag elements. Additionally, a graphical interface for steel/slag calculations that is easy to use and suitable for the steel industry has been developed. Such an interface, together with the TCOX database, is a powerful tool for controlling complex metallurgical processes, for example desulphurization, dephosphorization or ladle refining, and in the development of new steel grades.

In this paper several examples of applications of this new interface to simulate various aspects of the steelmaking process are presented.

## Introduction

Thermo-Calc has a very large and powerful thermodynamic database for oxide materials [1] that is -amongst many other possible applications- excellently suited for the calculation of reaction occurring during the steel making and steel refining process. The current version of the database (TCOX9, released in June 2019) now contains all the important elements for most steels, steelmaking slags and refractory materials (Fe-C-Co-Cr-Cu-Mn-Mo-Nb-Ni-V-W-Ti, Ca-Mg-Si-Al-F-O-P-S). Intensive development of the database is still under way and more elements are expected to be added in the near future as are models for molar volume, surface tension and viscosity.

In this paper we first touch on the conventional way in which thermodynamic equilibrium between the steel, slag and gas phase is calculated. We then present the TCOX9 database that is developed based on the CALPHAD methodology and use it together with a newly released Process Metallurgy Module to calculate examples of the following steelmaking and steel refining processes:

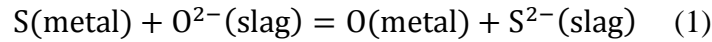
- Reactions taking place during converter steel making in the basic oxygen furnace (BOF).
- Deoxidation ("killing") of liquid steel by Si, Mn and / or Al addition on tap.
- Desulphurization using a CaO rich slag phase during steel refining in the LF.

- Transformation of Al<sub>2</sub>O<sub>3</sub> inclusions using CaSi wire addition during steel refining in the ladle furnace (LF).

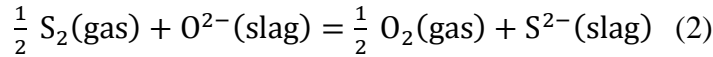
### Calculating steel – slag reactions based on equilibrium constants

Conventionally steel making and steel refining reactions are modeled using partition coefficients to determine how various elements are distributed between the liquid steel and the slag phase. These partition coefficients are calculated using equilibrium constants “K” that in turn require partial pressures and activities of solutes in the liquid steel and liquid slag phase. The well-known “sulphide capacity” model by Richardson and Fincham [2] is a good example of such a concept.

The partitioning of Sulphur between the liquid metal and the slag phase is given by the following exchange reaction.



Assuming the concentration of S and O in the liquid metal are the same as their partial pressure in the gas phase (which is probably correct at low oxygen partial pressures), we can re-write eq. 1 as follows.



The following equilibrium constant can then be defined for eq. 2:

$$K = \frac{a_{S^{2-}}}{a_{O^{2-}}} \cdot \sqrt{\frac{p_{O_2}}{p_{S_2}}} = \frac{f_{S^{2-}} \cdot \%S(\text{slag})}{a_{O^{2-}}} \cdot \sqrt{\frac{p_{O_2}}{p_{S_2}}} \quad (3)$$

Where  $a$  are the activities of S<sup>2-</sup> and O<sup>2-</sup> in the slag phase and  $p$  are the partial pressures of O<sub>2</sub> and S<sub>2</sub> in the gas phase. From this equation the important fact that low oxygen partial pressure increases the amount of sulphur in the slag phase becomes evident as a low oxygen partial pressure pushes the reaction in eq. 2 towards the right side. The S concentration in the slag phase can then further be defined by introducing the activity coefficient  $f$  of sulphur in the slag phase. This finally allows the definition of the sulphide capacity  $C_S$ :

$$C_S = \frac{K \cdot a_{O^{2-}}}{f_{S^{2-}}} = \text{wt}\% S(\text{slag}) \sqrt{\frac{p_{O_2}}{p_{S_2}}} \quad (4)$$

Then empirical relations between slag composition and the sulphide capacity can be made. One of the ones that is still widely used in the steel industry is the so called “optical basicity” that was derived by Sosinsky and Sommerville [3]. They introduce the term “optical”, as they correlate the spectral absorption of the slag with its ability to remove sulphur from the steel. This idea was probably inspired by the observation that “white” slags (rich in CaO with some Al<sub>2</sub>O<sub>3</sub>, MgO, SiO<sub>2</sub> but little else) were “good” and brown slags (the brown colour usually comes from a certain FeO content in the slag) were “bad”. This has been known since the early days of steelmaking and still today an experienced process metallurgist will be able to judge how good his slag is by taking a sample and observing its colour.

While concepts such as the sulphide capacity model have proven to be very useful, they have severe limitations. The most obvious one, is that some independent way of calculating the

oxygen and sulphur partial pressure is required. Without this information, eq. 4 is useless. The other limitation is of course that the sulphide capacity  $C_S$  must be empirically derived using experimental data for a certain composition and temperature range. Its usefulness will be very limited outside this range.

Using internally consistent thermodynamic databases developed using the CALPHAD method make concepts such as the one outlined above obsolete. With a software tool that allows the calculation of thermodynamic equilibrium at any composition, temperature and pressure by minimization of the Gibbs energy functions, such as Thermo-Calc, one can directly obtain the property one is interested in, such as for example the amount of Sulphur in the liquid steel. One can of course also easily obtain any other type of thermodynamic property, such as equilibrium constants, partition coefficients, chemical potentials, activities, activity coefficients, even heat capacity, enthalpy, phase fractions, solidus and liquidus temperatures, etc... should one wish to do so, as they are all direct results of partial derivatives or tangent constructions of the Gibbs energy functions.

### **CALPHAD Database for Oxide Systems: TCOX9**

During most steel making processes, the following phases are of central importance: the liquid steel phase, the liquid slag phase and the gas phase. In TCOX9 the Gibbs energy of the liquid phase is described using the ionic two-sublattice liquid model [4, 5]. This model allows the composition of the liquid phase to continuously change from metallic to oxidic. The liquid steel and the slag phase are thus described in a physically correct manner as one and the same phase (IONIC\_LIQUID) that can have different compositions that are separated by one or more miscibility gaps. In equilibrium all elements partition to either side of the miscibility gap. This means the concentration and activities of all elements in the liquid steel and the slag phase are automatically calculated in function of bulk composition, temperature, oxygen activity, etc... by the condition of thermodynamic equilibrium.

Apart from the liquid phase, TCOX9 contains all the solid oxide and sulfide phases that are relevant for secondary steel making, the major solid metallic phases and also a gas phase. This means that not only the composition of the liquid steel and slag phase can be calculated, but also the amounts and compositions of all other solid phases that might be present. It also means that most steel-making processes can be simulated using this single database.

The database has been developed using the well-established CALPHAD method using a huge number of different types of experimental data. The first version of the database was released in 1992, almost 30 years ago, but development of the database started even earlier. The database has been continuously expanded and improved by careful curation and validation ever since. Currently the database contains 382 phases and a total of 260 binary systems, 242 ternary system, 118 pseudo-ternary oxide systems and 32 oxy-fluoride and oxy-sulfide systems have been fully assessed. The reliability of the database in the multi-component composition space has been validated against thousands of experimental datapoints.

### **Thermo-Calc's Process Metallurgy Module**

Process metallurgy is basically all about judiciously controlling the temperature and the bulk composition of the steel and slag phase by additions of alloying element in the form of ferro-alloys, de-oxidizing agents such as Al or Si and slag formers or fluxing agents such as CaO, CaF<sub>2</sub> and others. Elements that are less noble than iron such as C or Si can be oxidized by blowing O<sub>2</sub> (gas) into the steel. C is oxidized to CO and escapes in the form of gas, Si is oxidized to SiO<sub>2</sub>, which is lighter than liquid steel and will float up and combine with the slag phase.

As outlined above all these reactions can be reliably calculated using Thermo-Calc and the database TCOX9. However -up to now- entering the composition of the whole steel + slag + gas system has been quite cumbersome, as the steel composition is usually given in weight % of elements, while the slag formers are defined in weight % of their components. Also the interpretation of the obtained results was quite tedious, as often 2 or more liquids (the liquid steel and one or more oxide liquids) and often several different solid oxides are obtained.

The workflow for the calculation of process metallurgy has been greatly simplified by the release of Thermo-Calc's Process Metallurgy Module that is available from Thermo-Calc version 2019b (released in June 2019) onwards. Figure 1 shows the Process Metallurgy Module GUI (this activity in Thermo-Calc is called Process Metallurgy Calculator) and some typical types of results that can be obtained. The first step is to setup the conditions for an equilibrium calculation. The calculator allows the definition of three basic types of material groups: steel, slag or gas. Within these groups any number of materials can be defined. An obvious choice of materials in a steel plant would be the compositions of all available scrap types, typical hot metal analyses and ferro alloys. All available slag additions could also be predefined. These can then be used for equilibrium calculations based on the steel grade specific steel-making recipe.

Three different types of calculations can then be performed: a single equilibrium calculation for the specific conditions that have been defined, 1-axis stepping calculation for any variable that has been defined, 2-axis mapping (or grid calculation) with two arbitrary variables. The fourth type of calculation is called "uncertainty" and could also be thought of as a sensitivity calculation. For this calculation type a maximum and minimum range is determined for one or several variables defined in the calculator. Thermo-Calc will then take samples within the defined range based on a gaussian distribution and will perform equilibrium calculations. This allows the user to investigate the sensitivity of a certain calculated property on one or several variables.

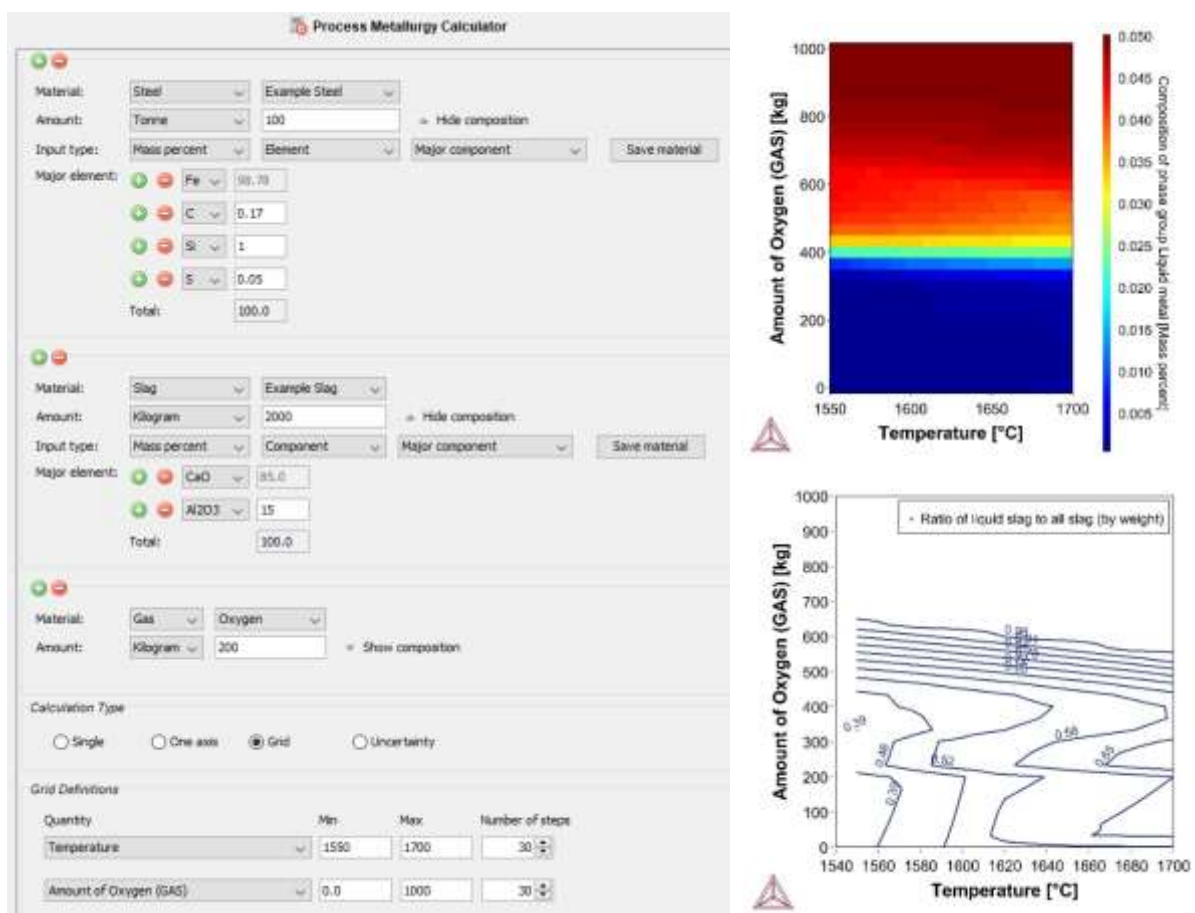


Figure 1. Setting up a steel - slag - gas equilibrium calculation with Thermo-Calc's Process Metallurgy Calculator (left) and typical plots showing equilibrium S content of liquid steel (top right) and fraction of liquid slag (bottom right)

## Example Calculations Using Thermo-Calc's Process Metallurgy Module

### Transformation Of Hot Metal To Steel In A Basic Oxygen Furnace (BOF)

In very simple terms, the principle of oxygen steelmaking in a converter is to blow oxygen into the carbon-rich hot metal coming from the blast furnace. The oxygen combines with the dissolved carbon to form CO which escapes as a gas phase. There are however many other reactions that occur simultaneously. We will take a closer look using the Process Metallurgy Module and the database TCOX9. We start by simply adding oxygen to 100 tonne of hot metal with the following composition, table 1. The calculation is performed isothermally at 1550°C.

Table 1. Initial composition of hot metal, wt%

Si	S	P	O	C	Mn	Al	Fe
1.00	0.04	0.12	0.003	4.50	1.00	0.03	Bal.

The plot on the left in figure 2 shows the evolution of phases in function of O<sub>2</sub> addition, the plot on the right shows the change in chemical composition of the liquid steel.

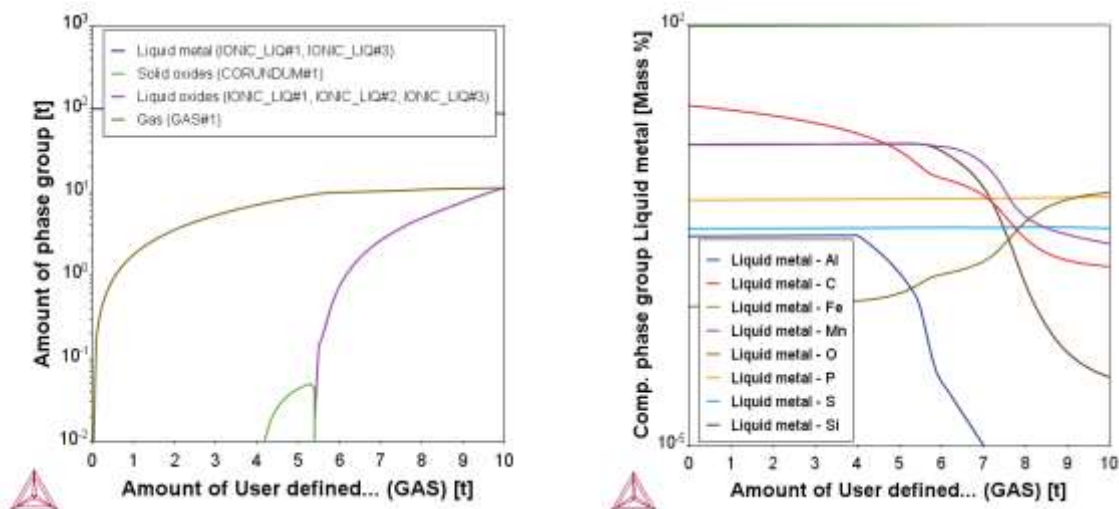
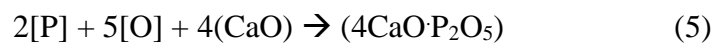


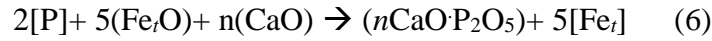
Figure 2. Evolution of oxide phases on adding O<sub>2</sub> to a typical hot metal composition (left) and evolution of the chemical composition of the hot metal on adding oxygen (right). Without addition of CaO rich slag former.

As expected the carbon content in the liquid steel decreases as it is oxidized to form CO gas. The content of other elements also decreases as they are oxidized to form solid or liquid oxide phases. But it can also be seen that there is no change in the S and P content of the liquid steel whatsoever. Both these elements are (in most cases) very detrimental to the final properties of the steel and they must be removed. But as they obviously cannot simply be oxidized, a different strategy must be employed.

In practice both S and P are removed from the liquid steel by transferring them to a CaO-rich slag phase by the following reactions.



or



and



Round brackets ( ) indicate elements dissolved in the slag phase and square brackets [ ] indicate elements dissolved in the liquid steel phase.

We now perform the same calculation as above, but we now add 3000 kg of slag former containing 85% CaO, 10% Al<sub>2</sub>O<sub>3</sub> and 5% MgO.

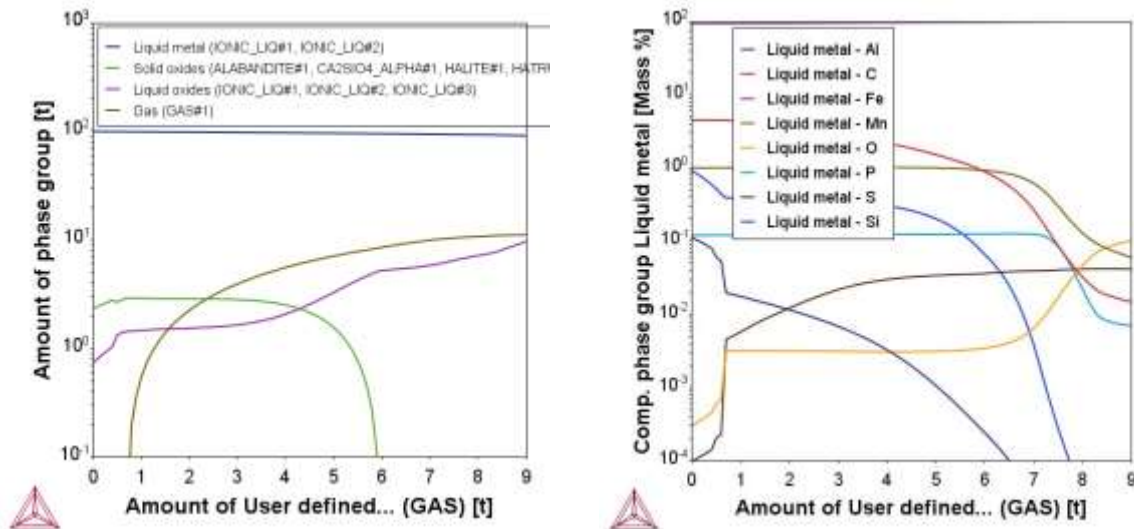


Figure 3. Evolution of oxide phases on adding O<sub>2</sub> to a typical hot metal composition (left) and evolution of the chemical composition of the hot metal on adding oxygen (right). With addition of 3000kg of CaO rich slag former.

We now find that the equilibrium P content in the liquid metal dramatically drops when more than 7 tonne of O<sub>2</sub> have been added to the system and as the oxygen content (and oxygen partial pressure) in the liquid steel starts increasing. That this should happen is evident from equations 5 and 6: increasing the oxygen content in the liquid steel pushes the equations towards the right side. P is removed by oxidation. For S on the other hand the opposite is true. Increasing the oxygen partial pressure in the liquid steel reverses the S out of the slag back into the steel. The important consequence is, that it is difficult to decrease the content of both S and P at the same time as they behave in opposite ways in function of oxygen partial pressure. The most common solution to this dilemma, is to remove P during steelmaking in the converter under oxidizing conditions and to remove S in a second steel refining step under reducing conditions.

### Deoxidizing (Or "Killing") Of The Steel On Tapping

As shown in the previous example, oxygen is used during steelmaking to oxidize and remove certain unwanted elements from the liquid metal. This is true in converter steel making where the high carbon content in the hot metal coming from the blast furnace must be removed. But it is also true in electric arc furnaces (EAF), where large amounts of oxygen are blown into the steel, not only to oxidize and remove certain elements from the liquid steel, but also due to the large amounts of energy released by these oxidation reactions that helps reduce the tap to tap time of the EAF.

The consequence is that liquid steel coming from a converter or EAF contains a large amount of dissolved oxygen, up to 1000 ppm or even more. On adding C, the most important alloying element in steel, the oxygen combines with the C forming CO gas. This results in a violent “boiling” reaction that causes severe operational problems. To prevent this, the steel needs to be de-oxidized or “killed”. This is typically done during tapping using Al or Si as de-oxidizing agents. These elements readily react with oxygen to form oxides that precipitate within the liquid steel. It should be noted, that this does not reduce the total amount of oxygen in the steel, it simply transforms the dissolved oxygen into an oxide precipitate. This oxide precipitate then needs to be removed from the steel by flotation. The oxides are lighter than steel and naturally float upwards. This upward motion is aided by purging the steel with Ar through porous plugs that are located in the bottom of the ladle.

Al is a very strong deoxidizing agent and very low values of dissolved oxygen can be achieved. The solid Al<sub>2</sub>O<sub>3</sub> that is formed has a plate-like morphology. The plates agglomerate to form large clusters that can be effectively removed by flotation. Si forms discrete solid SiO<sub>2</sub> particles that do not agglomerate and are difficult to remove. Therefore, Si is mostly added in combination with Mn as then an oxide liquid is formed, that is far less detrimental to the downstream casting process. Also the liquid precipitates tend to agglomerate to form large spherical oxides droplets that are more easily removed by flotation. As a rule of thumb, the Mn/Si ratio should be above 3:1 to assure liquid precipitate is formed. Often a combination of Si, Mn and Al is used for deoxidation. This results in lower dissolved oxygen in the liquid steel and if the right amount of Al is used it can result in a liquid inclusion. Too much Al will however lead to the formation of solid Al<sub>2</sub>O<sub>3</sub> (corundum) or Mullite.

With Thermo-Calc’s Process Metallurgy Module and the database TCOX9, it is very easy to calculate the amount and composition of oxides that are formed on killing a steel with any amount of dissolved oxygen using any combination of deoxidizing agents. Some simple examples of possible calculations are shown below using the following liquid steel composition, Table 2, that results from adding about 8000 kg of O<sub>2</sub> to the hot metal given in the previous section. Again 100 tonne of steel are assumed and the calculations are performed isothermally at 1600 °C.

Table 2. Steel composition during tapping from the converter after oxidizing with 8000 kg of O<sub>2</sub> together with 3000 kg of CaO rich slag.

Si	S	P	O	C	Mn	Al	Fe
0.00002	0.04	0.02	0.05	0.03	0.11	6e-7	Bal.

Figure 4 shows the dissolved oxygen in the liquid steel (blue contour lines) and the 90% liquid inclusion contour line (red) for no Al addition (left) and with addition of 20kg of Al (right). Such diagrams are very useful maps that can be used as guide for the most effective deoxidation method in function of the composition of tapped steel. These examples show, that without addition of Al, an dissolved oxygen content of about 100 ppm can be achieved. It can also be seen that for a Mn:Si ration of 3:1, liquid oxide precipitates are formed. If 20 kg of Al are added, much lower dissolved oxygen contents can be achieved. The calculations also show that the oxide precipitates are not purely liquid. Small amounts of solid Al<sub>2</sub>O<sub>3</sub> are also formed. Figure 5 shows how the composition of the liquid steel and also the oxide precipitate changes in function of increasing Si addition with Mn and Al additions kept constant at 450 kg and 30 kg respectively.

It should be noted, that other alloying elements are often also added at tap, in particular C. These additions will also have a profound influence on the killing reaction.

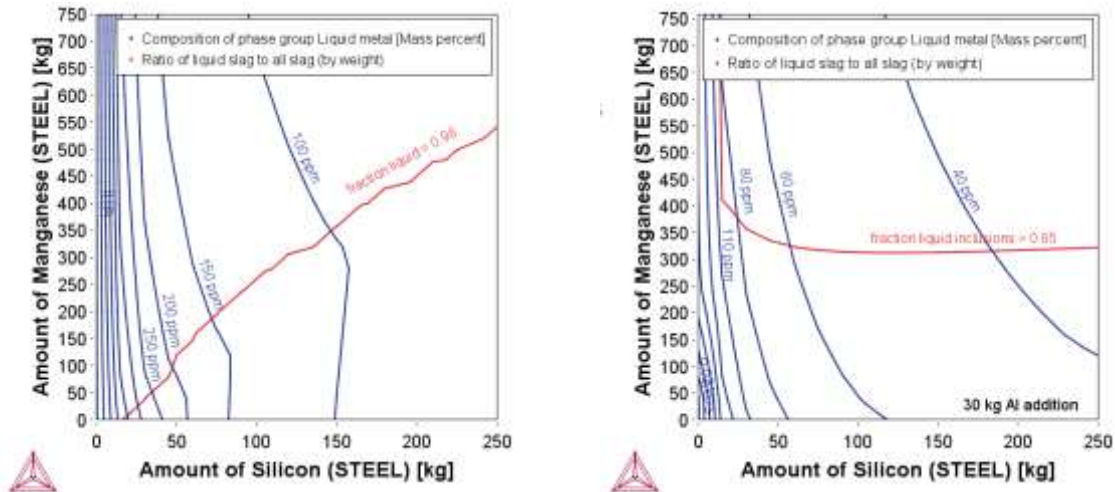


Figure 4. Dissolved oxygen in liquid steel (blue contour lines) and fraction of metal of liquid oxide inclusions (red contour line).

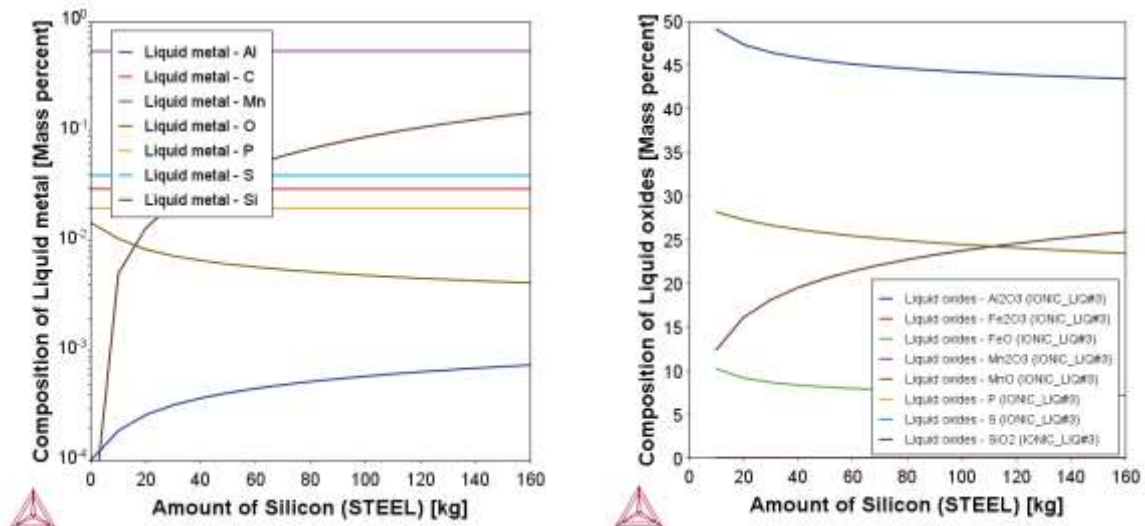


Figure 5 Liquid steel composition (left) and composition of liquid inclusions in function of Si addition. Temperature is fix at 1600°C. Fixed amounts of Al (30kg) and Mn (450 kg) are added.

### Desulphurization Using Steel – Slag Reaction In a Ladle Furnace

As previously shown, it is difficult to decrease the S content in the liquid steel during steelmaking as conditions are predominantly very oxidizing. Desulphurization is therefore usually performed during steel refining in a ladle furnace or a vacuum degasser after the steel has been fully killed by a suitable deoxidizing agent and the oxygen activity in the liquid steel is low.

Using the Process Metallurgy Module we take the steel given in Table 2 and add the following alloy additions: 200 kg Si, 500 kg Mn, 80 kg Al and 180 kg of C at 1600°C. These additions effectively de-oxidize the steel and result in the formation of ~100 kg of solid Al<sub>2</sub>O<sub>3</sub> precipitates. This would therefore be considered an Al-killed steel.

The resulting liquid steel composition given in table 3, that corresponds to a typical Al-killed 1020 grade, except for the S content, that is still considerably too high.



Table 3. Liquid steel composition after adding 200 kg Si, 500 kg Mn, 80 kg Al and 180 kg C at tap.

Si	S	P	O	C	Mn	Al	Fe
0.20	0.04	0.02	5 ppm	0.21	0.60	0.024	Bal.

Again using the Process Metallurgy Module, we will use this steel and calculate the equilibrium with a CaO rich slag phase with varying SiO<sub>2</sub> and Al<sub>2</sub>O<sub>3</sub> contents. For the de-sulphurization to be successful two conditions need to be fulfilled: 1) the slag must be fully liquid (liquid fraction > 0.9) and 2) the slag must take up a large amount of S from the liquid steel (have a “high sulphur capacity”) resulting in a low S content in the liquid steel. These two conditions are plotted as contour lines in figure 6. The plot on the right was calculated assuming some re-oxidation of the steel resulting in a FeO content in the slag of ~5 wt%. The most common reason for re-oxidation is carry over of FeO-rich furnace slag.

The ideal slag composition for de-sulphurization without re-oxidation is in a narrow band from 40% Al<sub>2</sub>O<sub>3</sub> and 0% SiO<sub>2</sub> to 20% Al<sub>2</sub>O<sub>3</sub> and 15% SiO<sub>2</sub>. With reoxidation this area is drastically reduced, meaning that de-sulphurization is much more difficult.

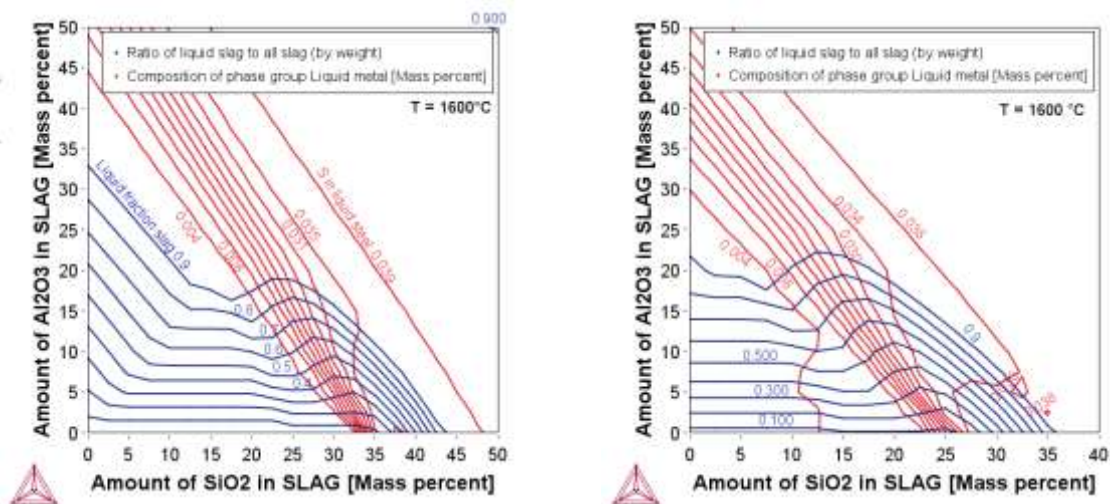


Figure 6. Equilibrium S content in the liquid steel (red contour lines) and liquid fraction of the slag phase (blue contour lines) for a slag with no FeO (left) and a slag with ~5wt% FeO acquired by re-oxidation by carry-over of furnace slag for example (right).

### Inclusion Modification By CaSi Wire Injection

The previous section outlined variations of Si deoxidation for the production of Si-killed steels. Al is a far more powerful deoxidation agent and much lower dissolved oxygen can be achieved. Al killed steels place special requirements on the subsequent continuous casting. The teeming stream from the ladle into the tundish must be protected from oxygen by a ladle shroud (LS) and the streams from the tundish into the moulds must be protected by a submerged entry nozzle or shroud (SEN or SES). Also, the steel surface in the mould must be protected from the atmosphere by applying mould powder. Often the LS, SEN and SES are also purged with Ar to make sure no re-oxidation and formation of oxide particles occurs. But even with all these measures, solid corundum (Al<sub>2</sub>O<sub>3</sub>) can still find its way into the mould, either because the Al<sub>2</sub>O<sub>3</sub> formed during killing of the steel is not fully removed by flotation during ladle treatment, or because small amounts of oxygen find its way into the liquid steel where it immediately combines with the dissolved Al to form Al<sub>2</sub>O<sub>3</sub>. Apart from being detrimental to the final steel product, Al<sub>2</sub>O<sub>3</sub> tends to stick to the tips of the stoppers used to control the amount of steel flowing from the tundish to the mould or to the inside of the SEN

and SES. This so-called nozzle clogging can result in premature termination of continuous casting resulting in loss of productivity and high operational costs.

A common practice in the refining of Al-killed steels is to add small amounts of calcium to the liquid steel towards the end of the refining cycle, by spooling a steel wire with a core of metallic Ca into the liquid steel. The  $\text{Al}_2\text{O}_3$  - CaO phase diagram shows that a low melting oxide liquid exists with a liquidus temperature below the typical ladle treatment temperatures at about 50 wt% CaO. This means that if just enough Ca is added to the liquid steel, all the solid  $\text{Al}_2\text{O}_3$  still present in the liquid steel can be transformed into a liquid oxide inclusion that is far less detrimental for the continuous casting process and also for the final application of the steel.

As mentioned in the previous sections the tapping additions resulting in the steel given in table 3 produces about 100 kg of solid  $\text{Al}_2\text{O}_3$  particles, that agglomerate in the liquid steel and are gradually removed during treatment in the ladle furnace by flotation. Ca treatment is done late in the refining process maybe 5-10 minutes before the ladle is sent to the continuous caster.

We calculate the CaSi treatment by taking the composition of the fully de-sulphurized steel in table 3 and add 20 kg of  $\text{Al}_2\text{O}_3$  corresponding to the assumed remaining oxides that have not yet been removed by flotation. We then add CaSi with a composition of 35 wt% Ca and 65 wt% Si. The plot on the right in figure 7 shows the evolution of solid oxide phases in the liquid steel in function of amount of CaSi added. Above an addition of 30 kg the inclusions are fully liquid.

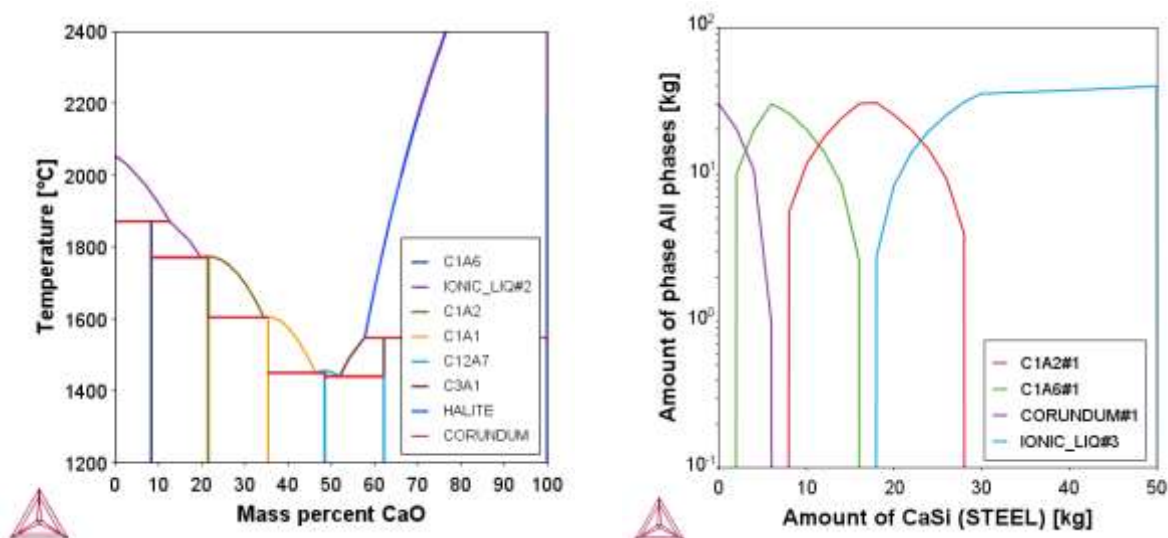


Figure 7. CaO -  $\text{Al}_2\text{O}_3$  phase diagram (left) and amounts of oxides in 100 tonne of liquid steel with initially 30 kg of  $\text{Al}_2\text{O}_3$  on adding CaSi wire (right).

### Conclusions And Outlook

Some example calculations for simple steel grades using Thermo-Calc's newly released Process Metallurgy Module and the oxide database TCOX9 have been presented. The examples roughly follow the actual process starting from steel making in a converter, deoxidation on tapping, desulphurization and finally inclusion modification by Ca treatment. This first release of the Process Metallurgy Module has the restriction, that only isothermal calculations are possible. In a future release, isenthalpic calculations will also be possible. This will allow the calculation of the actual temperature increase or decrease that occurs during additions. This will then for example allow the calculation of the temperature increase in a BOF converter due to the exothermic oxidation reactions happening.

The second restriction of the current release is that it only allows for equilibrium calculation. It is well known from plant experiments that all secondary metallurgy reactions are limited not only by thermodynamic equilibrium, but also by kinetics. Namely the heat and mass transfer to and from the phase interfaces where the reactions are occurring. There are simple but powerful kinetic models that take these effects into account, see for example [6]. It is also planned to implement such a kinetic model into the Process Metallurgy Module in the near future.

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