A Kinetic and Thermodynamic Description of the Steel Making Process using Thermo-Calc and the CALPHAD Database TCOX

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Summary

Internally consistent thermodynamic databases developed using the CALPHAD approach have continuously been expanded and improved for the last 30 years. The thermodynamic database TCOX9, that is to be released in June 2019, is well suited for calculating thermochemical interaction between liquid steel and slag during steel making and refining. It now contains all the major steel alloying elements (Fe-C-Co-Cr-Cu-Mn-Mo-Nb-Ni-V-W-Ti) as well as the most important slag elements (Ca-Mg-Si-Al-F-O-P-S) to be truly applicable to real-life industrial metallurgical processes. The liquid phase is modelled by the ionic liquid model, that describes the liquid phase over the whole composition range from metallic liquid (liquid steel) to oxide liquid (slag phase). The database also contains descriptions of the most important metallic and non-metallic solid phases, meaning inclusion formation, inclusion modification, steel solidification, slag solidification, steel-refractory reactions, slag-refractory reactions and steel-mould powder reactions can be calculated. It also contains a gas phase.

In part 1 of this paper some basic equilibrium calculations are presented (oxidation of steel, steel-slag interaction, oxide stability diagram for the Fe-Al-Ca-O system, calculation of Ca treatment). In part 2 a kinetic model of the steelmaking process is developed based on the concept of effective equilibrium reaction zone and applied to the processing of a simple Al killed steel grade with standard steel-making recipe.

This kinetic model can be employed by steel plants for off-line optimization of the day to day steel making practices or for the development steelmaking practices for new steel-grades. It can also be run in real time parallel to production using Level 2 plant data as part of the quality assurance system. Thermo-Calc's recently released application programming interface (API) based on Python programming language (TC-Python) is ideal for such applications.

Key Words

CALPHAD, thermodynamics, kinetic modeling, steelmaking, steel refining, inclusion modification, steel-slag interaction.

Introduction

Since many years Thermo-Calc has been well established in the field of physical metallurgy thanks to the very powerful and extensive steel database TCFE9. The diffusion add-on module DICTRA and more recently the precipitation module TC-PRISMA, have been extensively employed for applications ranging from nitriding and carburization to precipitation hardening. Until recently Thermo-Calc has been used less for process metallurgy, namely simulating the steel-making process involving steel-slag interactions, since a high-quality and reliable database of the oxide liquid (slag) phase, that contains all the important elements for steel processing was not available. This gap was closed when version 8 of the oxide database was released in June 2018, with the elements Co, Mo, P, V, W, Ar (only in gas phase) newly added [1]. The element Ti was added in the current version of the database (TCOX9, to be released in June 2019) and the database 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 in progress and further elements (Na, K, Li) are expected to be added in the near future. Development is also under way to include molar volume and viscosity data.

In this paper Thermo-Calc software and the database TCOX9 is used as calculation engine for a simple kinetic model, that has already successfully been employed to simulate the ladle furnace (LF) process [2][3][4], the basic oxygen converter (BOF) [5] and vacuum degassing (Ruhrstahl-Heraeus degasser) [6]. Here we combine all the process steps for the electric steel-making process starting from the scrap, melting in an electric arc furnace (EAF), tapping, refining in an LF and ending with the fully refined steel ready for casting on the continuous casting machine (CCM). Mass and heat balances are considered throughout the whole process: what goes in, must come out.

A common steel-grade is chosen (Al-killed SAE1020) that requires a rather simple steel-refining process. The model is set up with standard spread-sheet calculations and single point equilibrium calculations using Thermo-Calc and the database TCOX9. No programing skills whatsoever are required to reproduce the results. The model can be expanded and refined to describe the reactions in a more elaborate way, can be used for more advanced high alloyed steel-grades with more complex secondary steel-making routes and can be adapted to other steel-making process such as using hot metal or direct reduced iron as charge into the EAF or the reactions taking place in a basic oxygen furnace (BOF) and vacuum degasser. It can also be adapted to describe the stainless-steel making process including argon-oxygen decarburization (AOD) or vacuum-oxygen decarburization (VOD), etc...

The aim of this paper is to present the simplest possible model that still captures all the main reactions in a qualitatively correct manner throughout the whole process route:

- EAF: heating, melting, oxidation of C, Si, Al, de-phosphorization.
- Tapping: “killing” the steel, formation of non-metallic inclusions, alloying at tap.
- LF: temperature control, desulphurisation, removal of non-metallic inclusions, trimming, inclusion modification, Ca Treatment

It should provide a solid basis for the development of more elaborate models and it should also be easily possible to translate and expand it into software code using one of Thermo-Calc’s application programmer’s interfaces, such as TC-Python.

The TCOX8 Thermodynamic Database

The most important phase for the steel making process is the liquid phase. In TCOX9 the liquid is described using the ionic two-sublattice liquid model that was first introduced more than 30 year ago [7] [8]. This model allows the composition of the liquid phase to continuously change from metallic to oxidic. This allows the liquid steel and the slag phase to be described in a physically correct manner as one and the same phase (IONIC_LIQUID) that can have different compositions that are separated by a miscibility gap. In equilibrium all elements partition to either side of the miscibility gap, this means that concepts such as the sulfur capacity become obsolete, as 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 oxide and sulfide phases that are relevant for secondary steel making, the major solid metallic phases and also a gas phase. This means steel making can be modeled using this single database. For full description of steel solidification, the steels database TCFE9 should be used.

Equilibrium thermodynamic calculations of the steel-making process

Calculation 1: Oxidation of steel

Temperature control is key throughout the steelmaking process and therefore adiabatic calculations are far more useful than isothermal calculations (setting the enthalpy as condition instead of temperature), as this allows the calculation of the temperature change due to:

- exothermic reactions (typically oxidation by oxygen blowing)
- endothermic reactions (typically dissolution of alloys)
- cooling of the liquid steel by heat loss through the ladle or furnace refractory or off the top
- heat loss by hot gas escaping the furnace
- electrical energy input (electric arc)
- cooling effect of cold scrap or alloys being added to the system
- chemical energy from gas burners

It allows the answering of important questions such as how much energy can be saved in total by preheating the scrap to 400°C? Or how much electrical energy can be saved by increasing the oxygen blowing rate in the EAF?

As an illustration the reactions as a function of time under adiabatic conditions (meaning no heat flow into or out of the system) are calculated when oxygen (as O_2 gas at 15°C and 1 bar) is added to 100 t of steel with the initial composition given below.

Steel composition (amount 100t)

0.200 wt% C	0.023 wt% S	3E-5 wt% O
1.000 wt% Mn	0.250 wt% Si	Balance: Fe
0.025 wt% P	0.030 wt% Al	

This calculation could serve as an ideal model to illustrate the reactions taking place when O_2 is blown into or onto liquid steel in an EAF or BOF.

Figure 1 shows the sequence and amounts of phases that are formed and Figure 2 shows the temperature increase resulting from the exothermic oxidation reactions taking place. For these calculations it is assumed that 1 kg (0.75 Nm^3) of oxygen is added to the system per second. This corresponds to an oxygen flow rate of ~2700 Nm^3/h, which is a towards the top end oxygen flowrate for an EAF, but not exceptional.

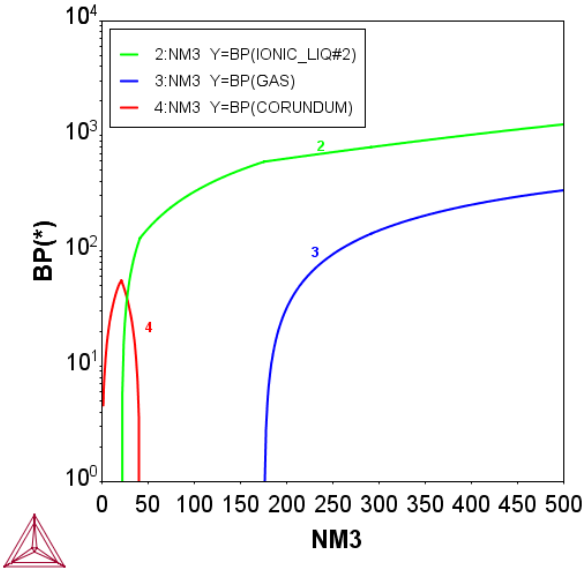

Figure 1. Evolution of phase fractions on adding oxygen to liquid steel. IONIC_LIQ#2 is the slag phase.

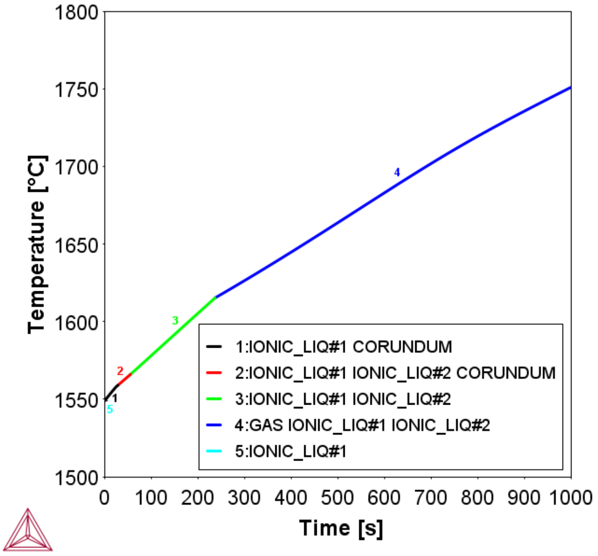

Figure 2. Temperature increase due to exothermic oxidation reactions on adding oxygen to liquid steel.

The amount of heat released by the exothermic reactions can be simply calculated as the derivative of the enthalpy of the liquid steel, H(ION#1).T in Thermo-Calc console mode syntax. This then would be considered as chemical energy input into the system and is shown in Figure 3. The equivalent power is quite substantial, ranging from 30 MW when highly exothermic reactions such as the oxidation of Al and Si take place, then reduces as these elements are depleted and less exothermic reactions take over. At the final stage almost all the power is due to the oxidation of Fe to FeO. It is interesting to note, that at the moment the oxidation of C starts, and a CO rich gas is produced, there is a drop in power. This is because considerable volume expansion work against atmospheric pressure is required (P*dV). Under vacuum conditions, the heat released by oxidation of C is significantly greater and the gas phase appears much sooner. This can easily be tested by repeating the calculation at a lower total pressure of say 1 Pa. Additional energy input into the furnace could be achieved by post-combustion of the CO gas to CO_2.

It should be noted, that this calculation is performed at equilibrium, meaning that infinitely fast mixing of the steel is assumed. In reality the steel close to the reaction site will be depleted. The kinetics of mass transport will severely limit the reaction rate and the theoretical power calculated here will not be reached. The reaction kinetics are addressed in the last section of this paper.

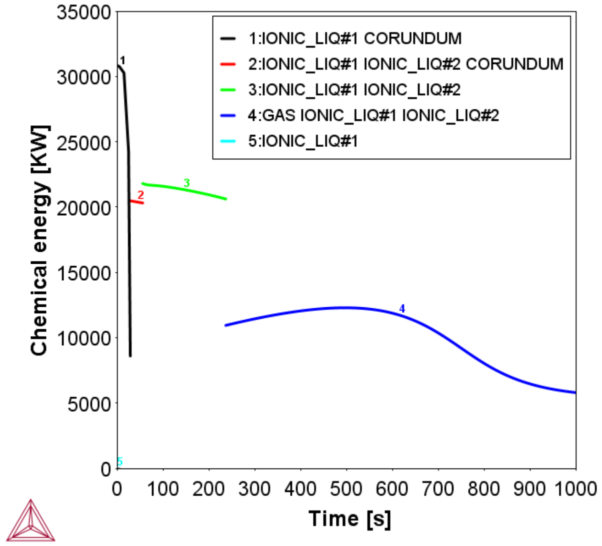

Figure 3. Chemical energy released by oxidation reaction on adding oxygen to liquid steel. IONIC_LIQ#1 is metallic liquid, IONIC_LIQ#2 is the slag phase.

The next key feature of steelmaking is the control of the steel chemistry. Figure 4 shows the change in steel chemistry on oxidation. Again 1 kg of oxygen is added per second. The well-known oxidation sequence as also shown in Ellingham diagrams is found with elements with high affinity to oxygen being oxidized first in the following sequence: (Ca) – Al – Si – C – Mn – (Fe). Once the element is oxidized it can be removed from the liquid steel into the slag phase by flotation (the oxide is always lighter than liquid steel) or as a gas bubble. It can also be seen that while there is a clear sequence, the reactions show considerable overlap, meaning that for example Mn is already starting to be oxidized before Al and Si have been fully oxidized.

The concentrations of P and S in the liquid steel on the other hand are largely unaffected by oxidation. Both P and S are in most cases undesirable and even for undemanding steel grades they should be below < 0.025 wt%, more demanding grades require P and S contents of < 0.01 wt% or even lower. These elements can obviously not be removed by simple oxidation as performed in *calculation 1* and a different strategy must be applied for their removal.

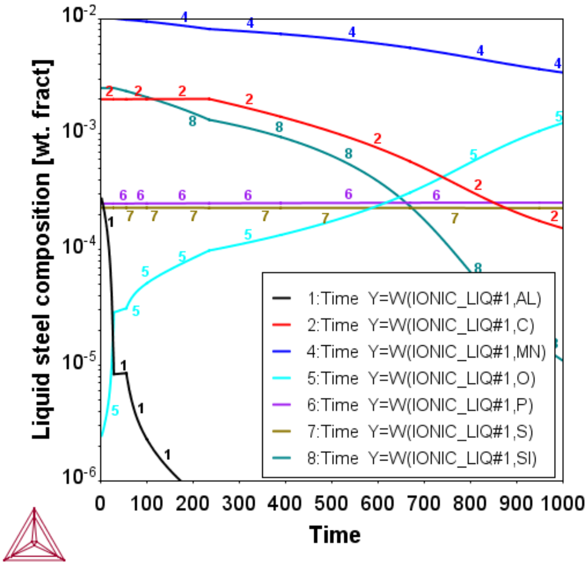

Figure 4. Evolution of the chemistry of liquid steel on oxygen addition. Composition given in weight fraction.

Calculation 2: Oxidation of steel + Ca-rich slag

In practice P and S are removed from liquid steel and transferred to the slag phase by the following reactions that involve a CaO – rich slag phase.

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

or

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

and

$(CaO) + [S] \rightarrow 2(CaS) + [O]$ Eq. 2

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

For this second calculation, oxygen is added to a system containing 100 t of steel plus 3 t of slag (30 kg lime per t of steel) with the following compositions:

Steel composition (amount 100 t)

0.170 wt% C	0.056 wt% S	1E-5 wt% O
0.900 wt% Mn	0.350 wt% Si	Balance: Fe
0.046 wt% P	0.040 wt% Al	

Initial slag composition (amount 3 t)

80 wt% CaO	10 wt% SiO2	10 wt% Al2O3

Note that the slag will become progressively richer in FeO and MnO as oxygen is added.

The oxygen flowrate is set at 2700 Nm^3/h which corresponds to 1kg of oxygen per second. The calculation is now performed isothermally at 1600°C. Again, this is an equilibrium calculation and infinitely fast mixing of the steel and slag to the reaction zone is assumed. Kinetics will be addressed in the last section of this paper.

Figure 5 shows a general challenge for steel-makers: Phosphorous removal requires oxidizing conditions, whereas sulfur removal requires reducing conditions. In general, and at atmospheric pressure, it is not possible to simultaneously remove sulfur and phosphorous. For the steel and slag chemistry investigated in this example, active oxygen must be *below* 10 ppm to be able to remove sulfur from the liquid steel and transfer it to the slag phase. For phosphorous removal active oxygen must be *above* 100 ppm.

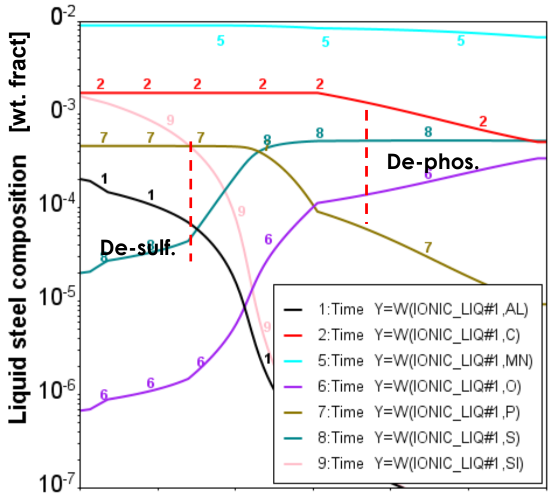

Figure 5. Evolution of the chemistry of liquid steel in equilibrium with CaO rich slag phase in function of oxygen addition.

This simple fact is the reason why the liquid steel is treated in two separate vessels, first in a steelmaking vessel such as an EAF or a BOF where oxidizing conditions prevail and then in a steel-refining vessel such as a ladle furnace, under reducing conditions. On tapping from the EAF or BOF into the ladle, oxygen in the liquid steel is removed (the steel is “killed”) by adding an element with a high affinity to oxygen. Al is used for Al-killed steels and Si or SiMn for Si-killed steels or some combination of both. The killing agent is typically added to the ladle during tapping to make sure that the killing agent is completely dissolved, and good mixing occurs. It also maximizes the available time for floatation of the formed oxides to the slag phase. It is vital that no slag phase from the furnace is tapped into the ladle, as this furnace slag has a high FeO content and thus a high oxygen activity and this will seriously impede the de-sulfurizaton in the ladle furnace.

Calculation 3: Inclusion modification

Apart from the chemistry control, the size, number and composition of the inclusions formed during the killing of the steel is of central importance. A very useful plot that is used to understand the nature of the non-metallic particles is the so-called oxide stability diagram, that can be constructed for many different deoxidizing systems. In Figure 6 the oxide stability diagram at 1600°C of the Fe-Al-Ca-O system that is relevant for Al killed steels with subsequent Ca treatment is shown.

The oxide stability diagram is not a true phase diagram but is a projection of different phase diagrams onto a common plane. It is basically equivalent to a liquidus projection, except that the temperature (a potential) is replaced with the oxygen potential. The fields show zero phase fraction regions of the stable oxide for the oxygen potential corresponding to a given oxygen content in the liquid steel. The sequence of phases that form corresponds to the phases in the CaO – Al_2O_3 phase diagram (Figure 8). An excellent review of these very useful diagrams has recently been published by Kang and Jung [9]. Their paper also contains a very clear step by step instruction on how such diagrams can be calculated with a software such as Thermo-Calc or others that use Gibbs energy minimization based on the CALPHAD method.

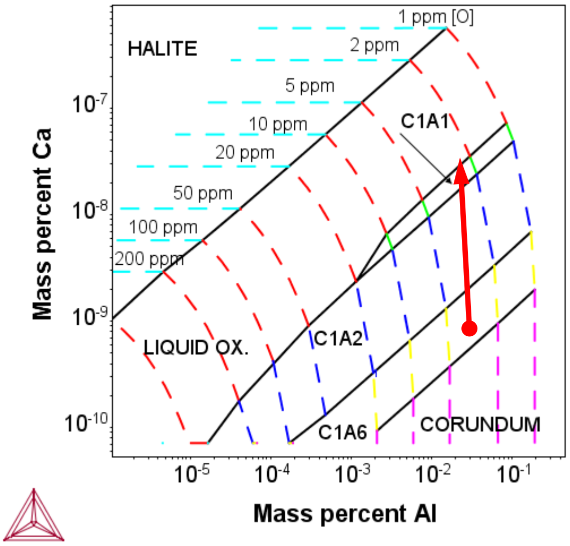

Figure 6. Oxide stability diagram of the Fe-Al-Ca-O system at 1600°C in function of Al and Ca dissolved in the liquid steel. Oxygen dissolved in the liquid steel is shown as dashed lines. The red arrow shows the composition change due to Ca treatment shown in Figure 7.

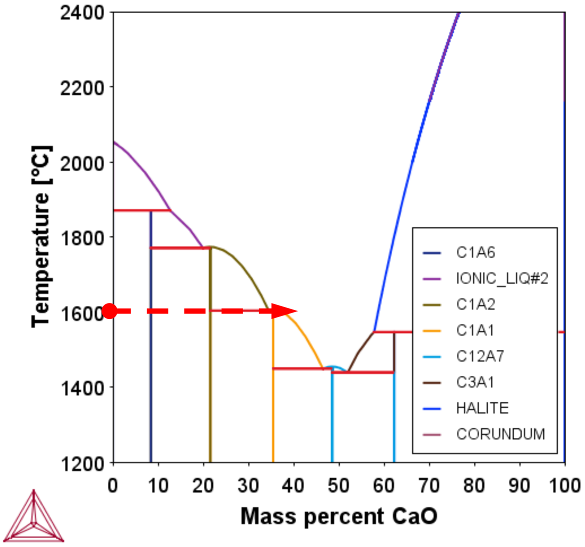

Figure 7. CaO-Al_2O_3 phase diagram calculated using the database TCOX8. Ca treatment transforms the Al_2O_3 inclusions into oxide liquid as indicated by the red arrow.

Calculation 4: Ca treatment

The main oxide formed in Al-killed steels is Al_2O_3 (corundum). This phase can agglomerate and cause serious operational problems during continuous casting (nozzle clogging). The solid Al_2O_3 can be transformed into liquid oxide inclusions by Ca treatment. In this process, a wire with a steel mantle and a core of metallic Ca is spooled into the steel. The oxide stability map shown in the previous section (Figure 6) gives a clear overview on the general phase relations, however it does not quantify how much Ca is required to transform all the Al_2O_3. If the complete steel chemistry and amount of inclusions in the steel is known at the time when Ca treatment is to be performed, a 1-axis stepping calculation will give a quantitative prediction of how much Ca is required to fully transform the Al_2O_3 inclusions to liquid oxides. Kinetically modeling the steelmaking process (see next section) gives exactly this information. In Figure 8 the phase evolution in the liquid steel with the chemistry and inclusion content after 20 min of LF treatment, as calculated with the kinetic model presented in the next section, is plotted in function of Ca addition. For this case, 6 kg of Ca is adequate to transform all the solid Al_2O_3 in the steel into liquid oxide inclusions (IONIC_LIQ#2). The amount of Ca that is required varies dramatically in function of steel chemistry and inclusion content. If Ca treatment is done earlier in the LF process more Ca will be required as more Al_2O_3 is still in the steel. Also, the steel still contains more S and Ca will be consumed to form sulfide phases and will not transform the Al_2O_3. Considerable quantities of Ca can be lost due to evaporation during wire feeding and operational skill and experience is required to maximize the Ca yield by optimizing the wire feeding speed and entry angle. Here a yield of 100% is assumed, which can surely not be achieved in practice.

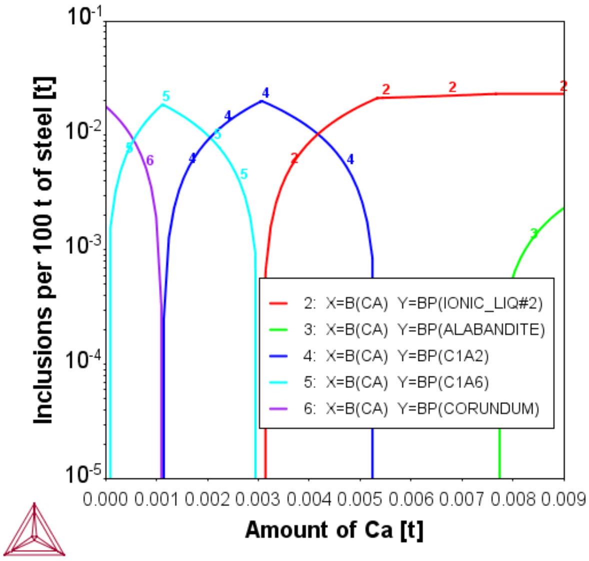

Figure 8. Transformation of Al_2O_3 inclusions after 20min of LF treatment as a function of Ca addition. A very small addition of 6 kg is required to fully transform all the Al_2O_3 into liquid oxide inclusions (IONIC_LIQ#2).

A kinetic model for the steel-making process

The preceding calculations assumed equilibrium throughout the bulk of the steel and slag phase and are very useful to gain basic insights. In reality steelmaking is also governed by kinetics as gradients in composition and temperature are present throughout the process.

Local equilibrium at the phase interfaces is however established. This means thermodynamic equilibrium determines where the reactions are headed and reaction kinetics (heat and mass transfer rates) determine how fast equilibrium is approached.

A simple but powerful way to combine kinetic effects with thermodynamic equilibrium calculations, that has been widely used to simulate the steelmaking process [2-6] has come to be known as the effective equilibrium reaction zone (EERZ) model. The principle of this model is outlined in Figure 8. The numbers in the figure correspond to the following steps.

1. Heat and mass transfer into the EERZ from the bulk of the liquid steel and slag phase.
2. Calculation of the thermodynamic steel-slag equilibrium within EERZ. The temperature homogenizes and the amount of steel and slag and their compositions assume the equilibrium values, meaning that mass transfer occurs across the steel-slag interface.
3. Heat and mass transfer out of the EERZ into the bulk of the liquid steel and slag phase.
4. Homogenization of the bulk liquid steel and slag phase.

The reaction kinetics are modelled with the size of the EERZ. If is the same size as the whole system, then reaction kinetics are infinitely fast and equilibrium between steel and slag is immediately achieved. This is the case in the equilibrium calculations presented in the preceding section. In reality the kinetics are governed by mass transfer to and from the reaction interface. Slow kinetics can be simulated by choosing a small EERZ faster kinetics are obtained with a larger EERZ. The size of the EERZ is therefore a fitting parameter for the reaction kinetics. The size of the EERZ could be calculated using empirical mass transfer equations similar to the ones given by Harada *et al.* [3] that consider parameters such as bath area, stirring intensity, steel and slag viscosity, etc…

The EERZ size and time-step length are linked. The only "free" model parameter is the reaction rate of the interface reaction (typically called "K" with units mass per time) and is defined by

$$K = (rho \cdot V) / t$$

where rho is the steel density, V is the volume transferred across the interface and t is the time-step. A long timestep requires a large EERZ, but the length of the timestep should -in principle- not influence the result.

Heat and mass balance must of course be strictly enforced in the mode.

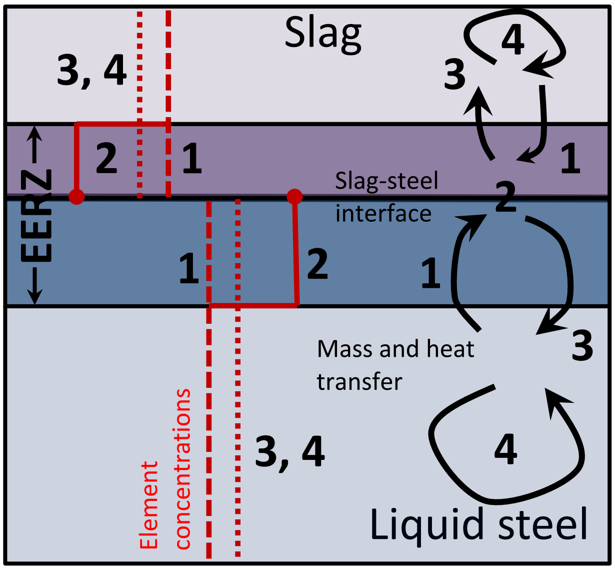

Figure 9. Schematic of the kinetic model, details see text.

Despite its simplicity this model turns out to be very powerful. In this paper it has been implemented in the simplest possible form. For a more quantitatively correct description of the steelmaking process, it can be expanded to consider other reactions such as refractory erosion or alloy dissolution.

Kinetic steel-making model for Al-killed grade 1020 for the scrap – EAF – LF process

In the following a kinetic model is outlined for the steelmaking process from scrap to refined steel in the EAF – LF process for the Al killed grade 1020 including Ca treatment.

A typical steel-making recipe for a plant with 100 t tapping weight, a 60 MW EAF with gas burners producing an additional ~10 MW of power, oxygen lance, carbon and lime injection. The gas burners were accounted for simply with an energy addition. The actual chemical reaction taking place in the burners and the influence of the burners on the furnace atmosphere could also be modeled, however this would require appending a database that contains a gas phase with hydrogen, such as SSUB6. All calculations were performed one-by-one with a timestep of 5 min in a spreadsheet.

The main features of the implemented model are as follows:

- Considered elements: Fe, C, Mn, P, S, Si, Al, O.
- Apart from the liquid steel and slag phase, all other stable metallic and nonmetallic solid phases and also the gas phase are considered in equilibrium calculations.
- Full mass and energy balance is strictly enforced: Everything entering the furnace (alloys, gas, heat, etc…) and everything leaving the furnace (gas, heat) is accounted for.
- Steel – slag interaction is modeled using the EERZ model with 5 min time-steps. In the EAF the EERZ is taken as 20-35% of the steel amount and 15-20% of the slag amount. In the LF, where reactions are less violent, the EERZ size is 20% of the steel amount and 15% of the slag amount. For a shorter time-step a smaller size must be chosen.
- 100% of injected matter (oxygen, carbon, lime) enters the EERZ and is homogenized. Bulk alloy additions are assumed to dissolve and be homogenized in the liquid steel phase within one timestep, bulk slag additions (Lime) are assumed to homogenize in the slag phase in one time-step. Especially the latter assumption might not be realistic. Incomplete homogenization could easily be introduced as an additional parameter in a more sophisticated model.
- All calculations performed adiabatically (not isothermally) meaning that the temperature increase or decrease by heating, cooling, alloy additions, exothermic oxidation reactions, etc, are quantitatively accounted for.
- The energy and components (mainly CO/CO2, but also small amounts of S and P) removed by the gas phase are fully accounted for.
- No mass exchange between the steel / slag and the furnace shell or ladle refractory (refractory erosion) is considered.
- The heat loss through the furnace shell or ladle wall and the heat transfer from the electric arc to the slag and steel is estimated. Net energy input by electric arc and gas burner in the EAF is 11.5 to 17.5 GJ per 5 min timestep (~40 – 60 KW average). In the LF it is between zero and 1.2 GJ per 5 min time-step.

The following steel-making recipe was implemented:

EAF process:

Time 0: 10 t of hot heel and 0.4 t of furnace slag (both 1600°C) already in furnace. First scrap bucket with 35t of scrap #1 (bundles), 15 t of scrap #2 (turnings) and 0.5 t lime charged to the furnace. Note that unusually high P and S content in the scrap is assumed to highlight the P removal in the EAF and S removal in the LF. Lime is kept very low to highlight the P removal by lime injection.

Time 20 min: Second scrap bucket with 35 t of scrap #1, 15 t of scrap #2 and 0.2 t lime charged to the furnace.

Electric arc power, carbon, lime and oxygen injection profiles are shown in Figure 9. Average over 5 min timesteps is shown. Of course, power and burners are off during actual charging of the second bucket (2-3 min).

Tapping additions:

100 t of steel is tapped from the EAF into the ladle with 0.1 t slag carry-over. About 1 t of the charged scrap is oxidized meaning that only 9t of hot heel is left. But the overall mass is conserved: what goes in must come out. Tapping additions: 0.15 t FeSi, 0.6 t FeMn, 0.15 t Al, 0.15 t C, 0.5 t lime.

LF process:

15 kg of CaSi wire added 20 min after tapping. Ar bubbling is assumed resulting in 10 – 30 % of the inclusions being transferred from the liquid steel to the slag phase per 5 min time-step. Electric arc power profile is shown in Figure 9.

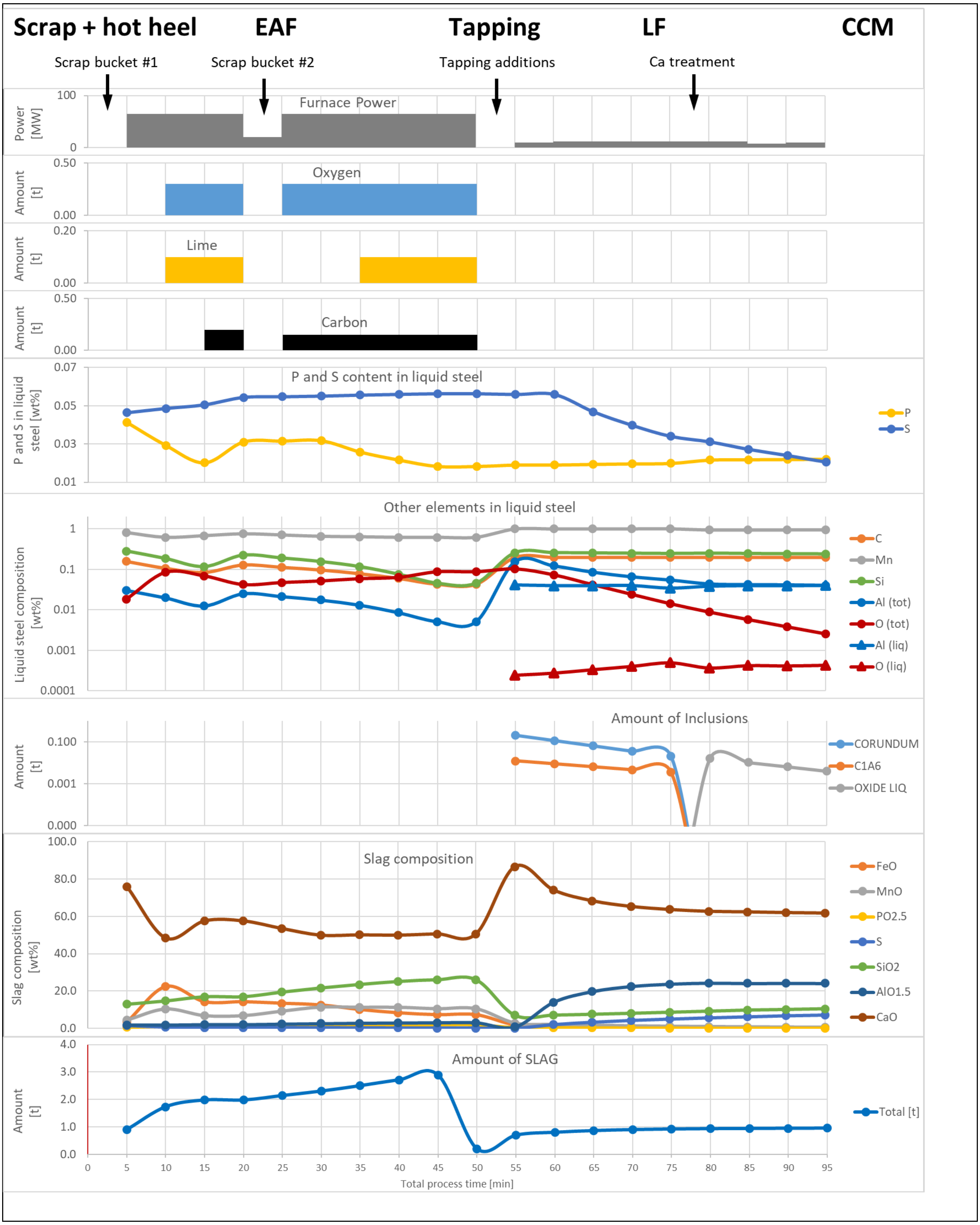

Figure 10 . Results of the full kinetic simulation of the steelmaking process from scrap to final refined steel ready for casting on the CCM. The arrows show times at which material is charged to the furnace (for details of additions see text). The bars at the top of the figure show furnace power in function of time and additions by injection (given in t per 5 min timestep). Al(tot) and O(tot) are total aluminium and oxygen in the steel, i.e. the sum of Al and O bound in the form of oxide inclusions plus Al and O dissolved in the liquid steel (Al(liq), O(liq)).

Results

Some selected results from the simulation are shown in Figure 9 The following quantities can be obtained from the simulation in function of time:

- Composition of the liquid steel, activity of all components in the steel.
- Type, amount and composition of inclusions.
- Amount and composition of furnace and ladle slag phase.
- Amount and composition of the gas phase.
- Temperature.
- Derived properties such as slag basicity, slag sulfur capacity, oxygen activity, dissolved oxygen, total oxygen, etc…
- The energy, alloy and gas consumption per ton of steel produced.

The final steel chemistry obtained is

0.198 wt%C, 0.95 wt% Mn, 0.022 wt% P, 0.018 wt% S, 0.24 wt% Si, 0.04 wt% Al. Total oxygen is 16 ppm which is within the specification of this particular steel grade.

Conclusion and outlook

This paper presents some very basic concept and calculations of the steel making process using the Thermo-Calc and the database TCOX9. All models and calculations are kept at the simplest possible level while still capturing the main essence of all the thermodynamic and kinetic processes occurring during steel-making process. These are

- Dephosphorization and desulfurization in function of time.
- Quantification of inclusion type and composition in function of time.
- Inclusion modification or engineering.
- Energy balance during the whole steel-making process under full consideration of the composition and temperature of all charge materials and the chemical energy released by exothermic oxidation reactions.

The calculations outlined can be easily reproduced with basic knowledge of Thermo-Calc and without any programming experience whatsoever. These concepts can thus be used as a starting point of more elaborate models including other kinetic effects or more elements and more complex steel-grades. Also, by comparing with real data from steel-plant operation, the model parameters can be adjusted to achieve quantitatively correct results.

The model can be implemented in software code using for example TC-Python. This opens the door to many very powerful opportunities, such as fitting the model parameters to experimental data, implementing smaller timesteps, introducing additional complexity to the model, etc… It would also allow the optimization of the steel-making process with regard to one or several parameters such as steel cleanness, sulfur content or even -and probably most importantly- minimized total cost of steel production.

Finally, it could also be envisaged that such a model could be run in parallel to the steel production in real time using process data taken from the steel plant Level 2 automation system and compared to samples taken during production. This would be a very powerful tool for process optimization and quality assurance of day to day production.

Abbreviations

CALPHAD: Originally an acronym for "CALculation of PHAse Diagrams. Now understood as "Computer Coupling of Phase Diagrams and Thermochemistry".

EERZ: Effective equilibrium reaction zone.

EAF: Electric arc furnace.

BOF: Basic oxygen furnace.

LF: Ladle furnace.

AOD: Argon-oxygen decarburizer.

VOD: Vacuum-oxygen decarburizer.

CCM: Continuous casting machine

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