Thermo-Calc Software

The application of an effective equilibrium reaction zone model based on CALPHAD thermodynamics to steel making

or

The story of Thermo-Calc's Process Metallurgy Module

Paul Mason, A. Nicholas Grundy, Ralf Rettig, Lina Kjellqvist,
Johan Jeppsson and Johan Bratberg

Thermo-Calc Software

Thermo-Calc Software

- Company dedicated to provide computational tools in the field of materials engineering
- Phase diagrams, thermodynamics, diffusion, kinetics of phase formation / transformation
- Founded in 1997
- Headquarters in Stockholm
- Total of ~40 employees worldwide
- > 1250 customers in 70+ countries

CALPHAD databases

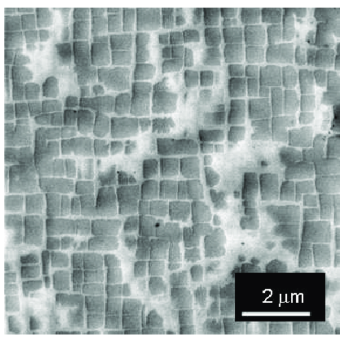
Thermo-Calc Software

Steel, cemented carbides,
High Mn, stainless

Aluminium alloys
Magnesium alloys

Titanium and Ti-Aluminides

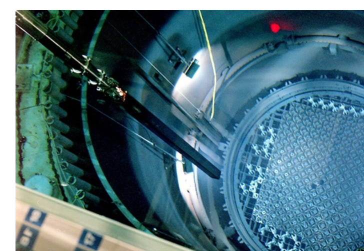
Aqueous, corrosion



Nickel superalloys

Nobel metals

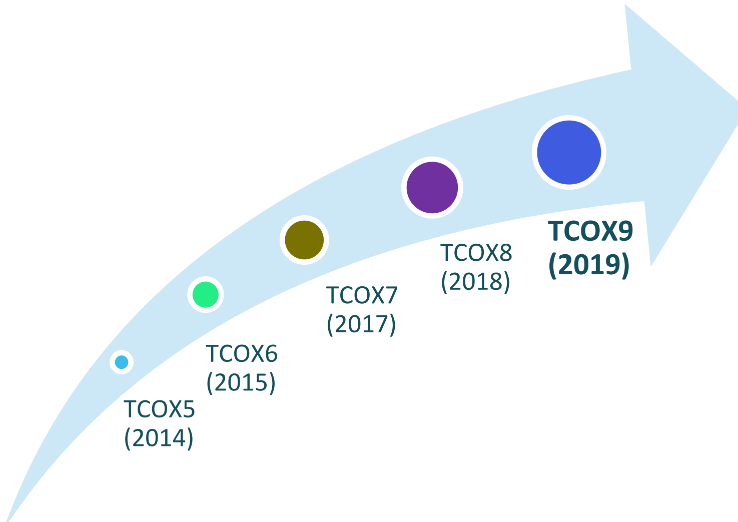
Also High Entropy Alloys, Copper alloys, Pure Silicon,
Molten salts, solder materials, and…..



Nuclear materials

CALPHAD Database for Oxides: TCOX9

Thermo-Calc Software



- ❑ 25 elements
- ❑ 260 binaries
- ❑ 244 ternaries
- ❑ 118 pseudo-ternary MeO-MeO-MeO
- ❑ 32 Me-O-F, Me-O-S
- ❑ Many higher order systems
- ❑ Validation in multicomponent space

From Dec 2019 also physical properties (viscosity, surface tension, density)

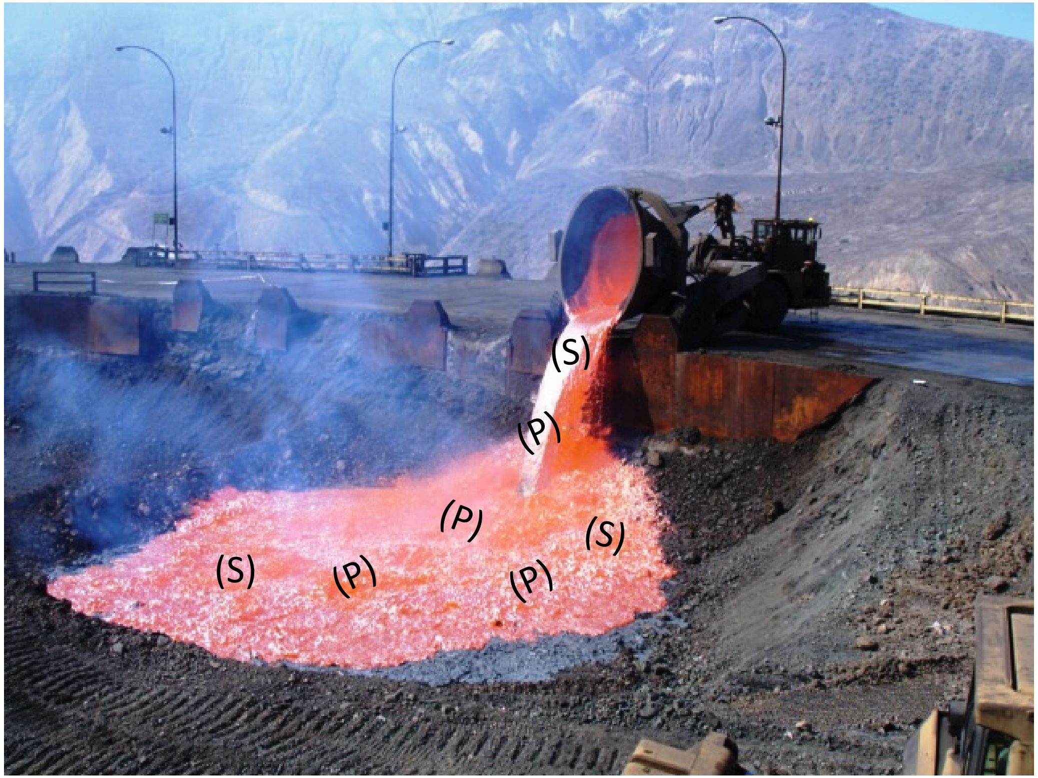
Al	Ar	C	Ca	Co	Cr	Cu	F	Fe
Gd	La	Mg	Mn	Mo	Nb	Ni	O	P
S	Si	Ti	V	W	Y	Zr		

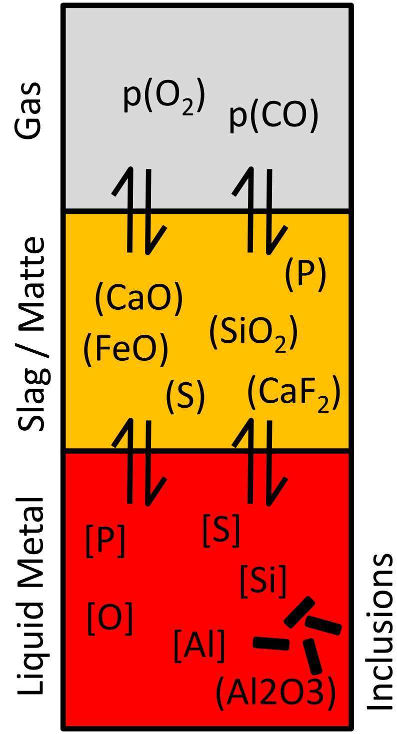
Details of database development under www.thermocalc.com

CALPHAD Database for Oxides: TCOX9

Thermo-Calc Software

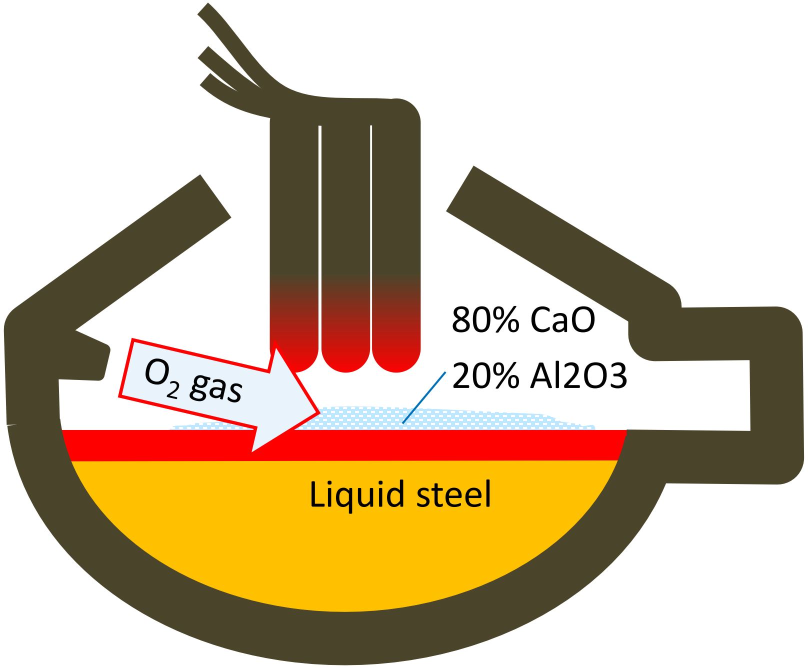
Replaces SLAG database
For process metallurgy (and many other things)





Applications of TCOX9

Thermo-Calc Software



$2[P] + 5[O] \rightarrow (P_2O_5)$ or

$2[P] + 5(FeO) + 4(CaO) \rightarrow (Ca_4P_2O_9) + 5[Fe]$

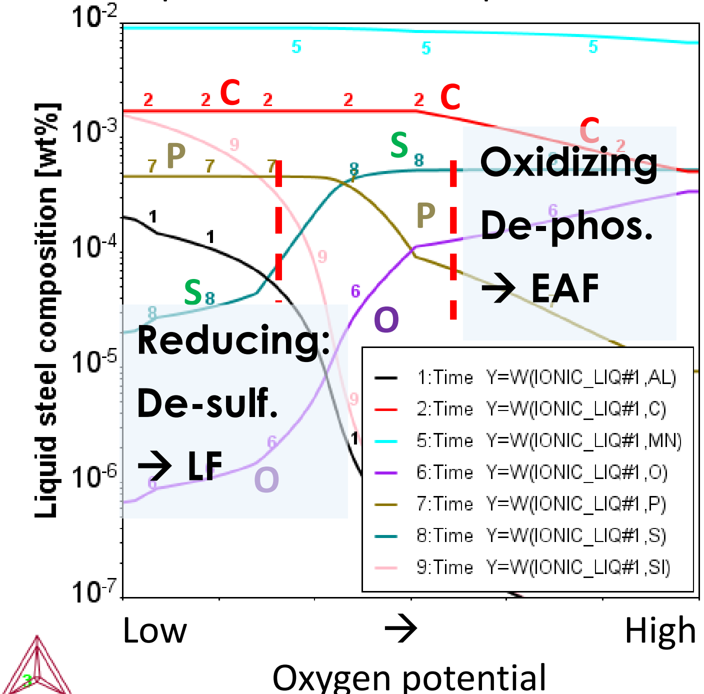
→ **Oxidizing conditions!**

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

→ **Reducing conditions!**

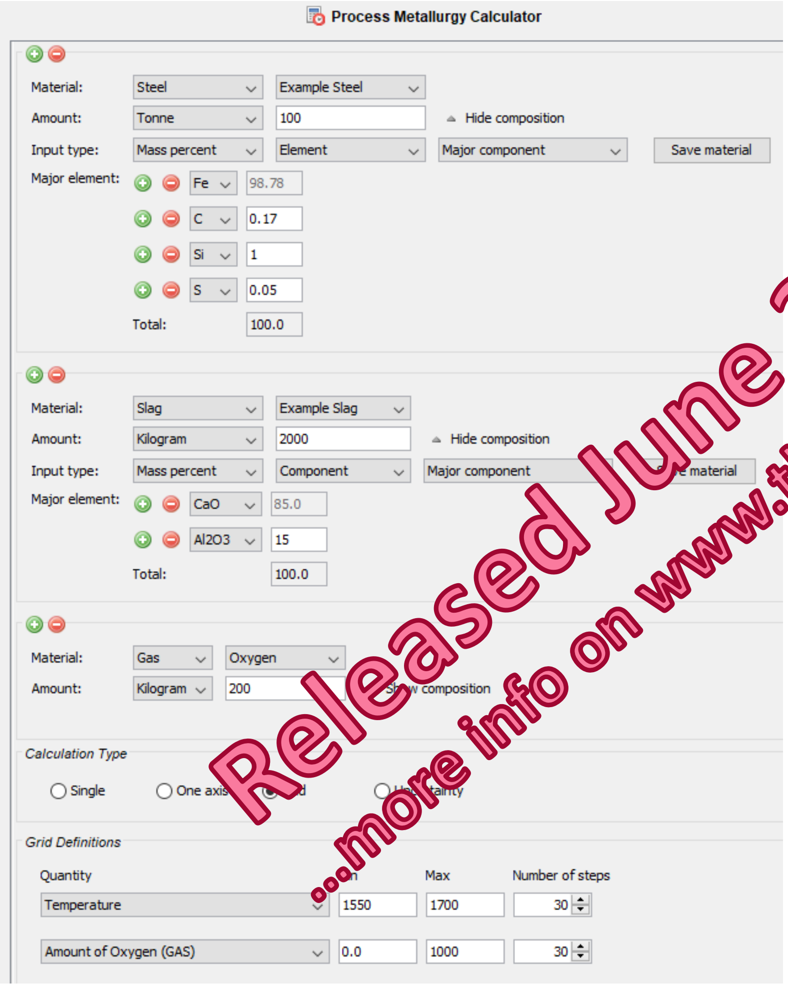
→ Isothermal calculations

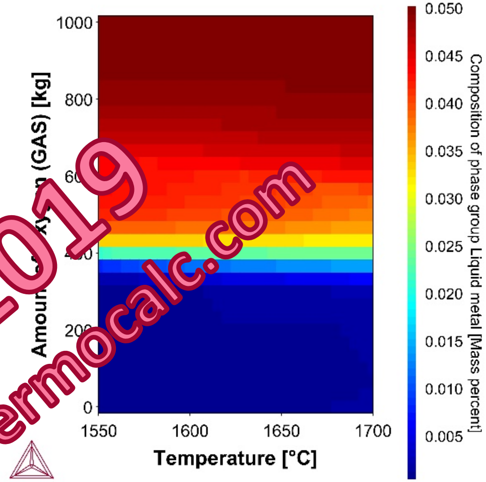
Equilibrium steel composition

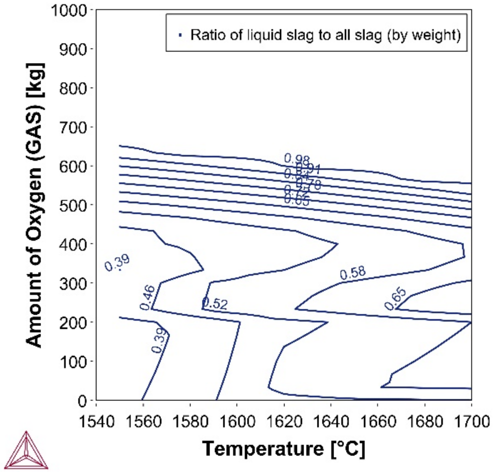


New easy to use interface to set-up steel-slag calculations

Thermo-Calc Software

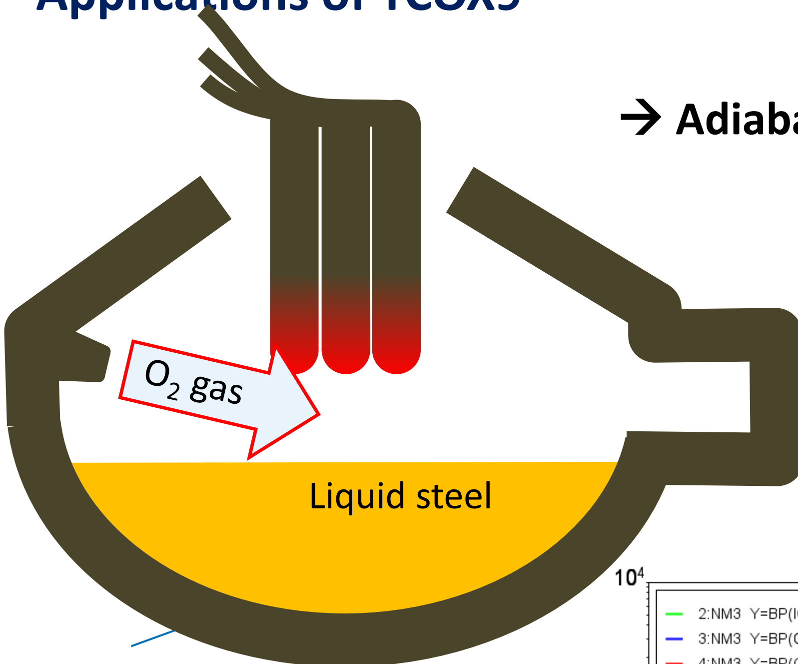




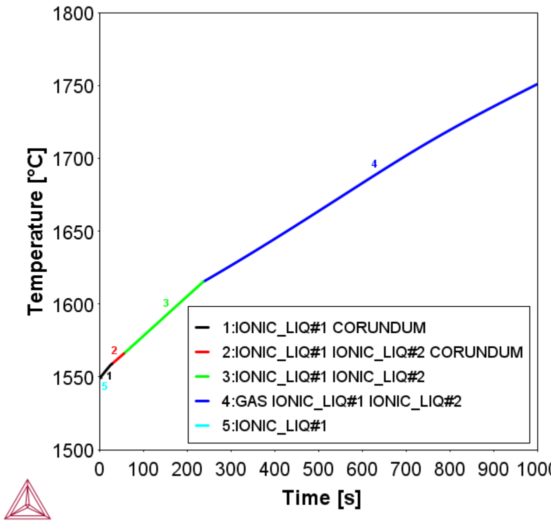


Released June 2019
...more info on www.thermocalc.com

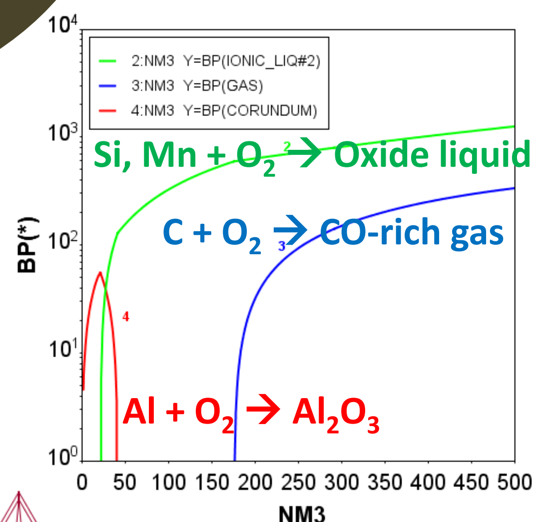
Applications of TCOX9

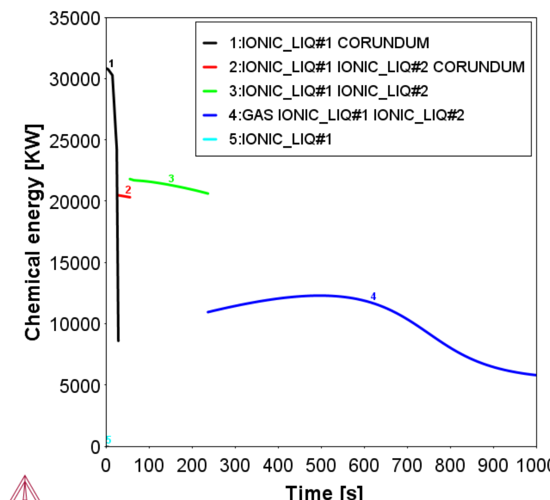


→ **Adiabatic calculations**



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

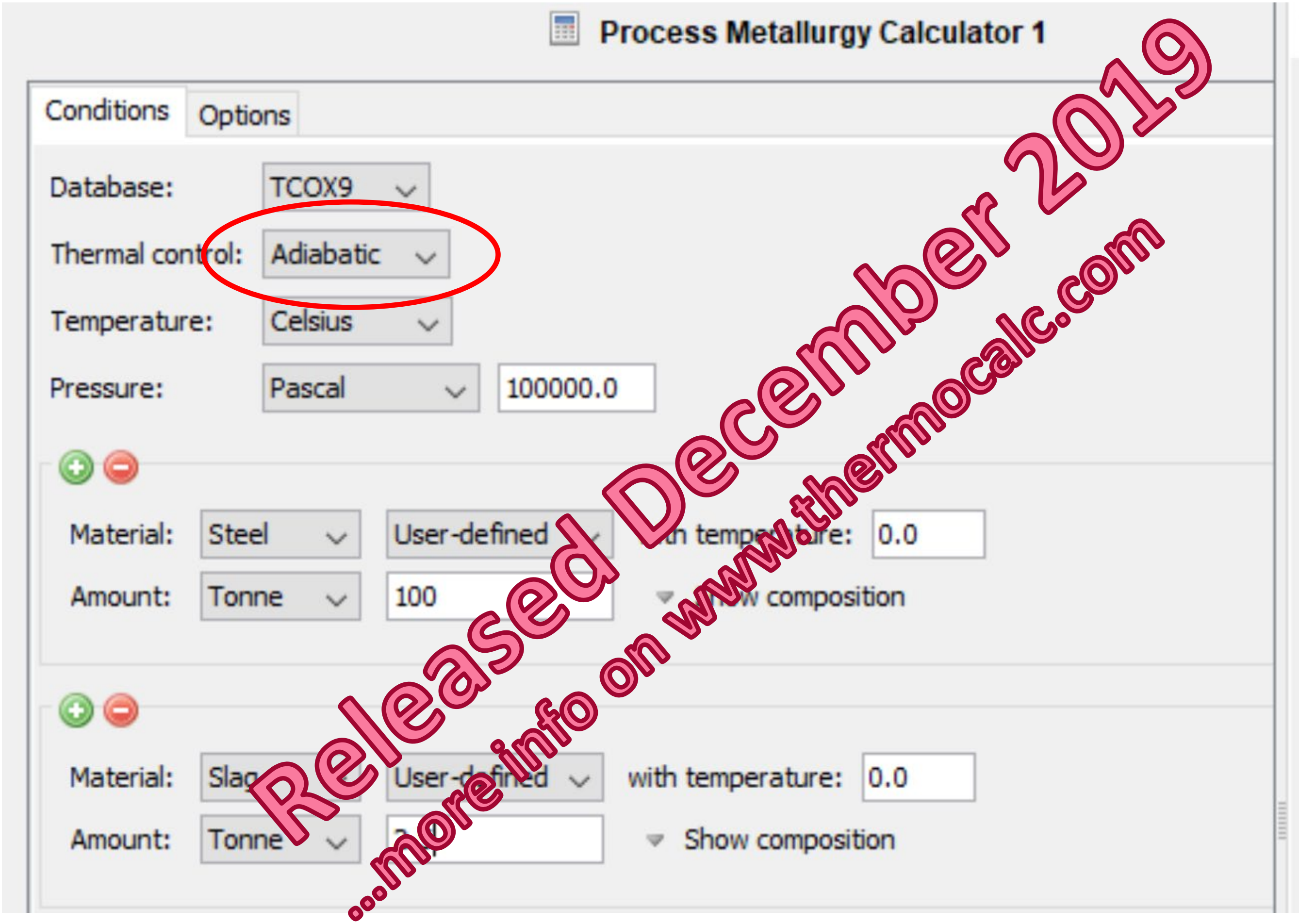




THE WORLD COMES HERE TMS2020 149th Annual Meeting & Exhibition
CO-LOCATED INTERNATIONAL CONFERENCE PbZn 2020

New easy to use interface to set-up steel-slag calculations

Thermo-Calc Software



Thermo-Calc Software

(

Applications for adiabatic calculations

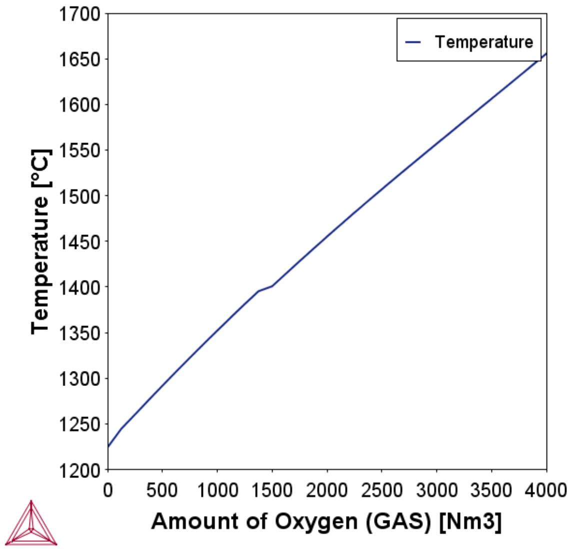
→ **Example 1 in Thermo-Calc help**

Steelmaking in a BOF converter:

C (in steel) + O_2 → CO_2

Or

2 C + O_2 → 2 CO



THE WORLD COMES HERE
TMS 2020
149th Annual Meeting & Exhibition
CO-LOCATED INTERNATIONAL CONFERENCE
PbZn 2020
February 23-27, 2020
San Diego, California, USA
#TMSAnnualMeeting

Thermo-Calc Software

Applications for adiabatic calculations

→ Real requests coming from customers!

Thermite welding process:

Al + FeO → Fe (liq) + Al2O3

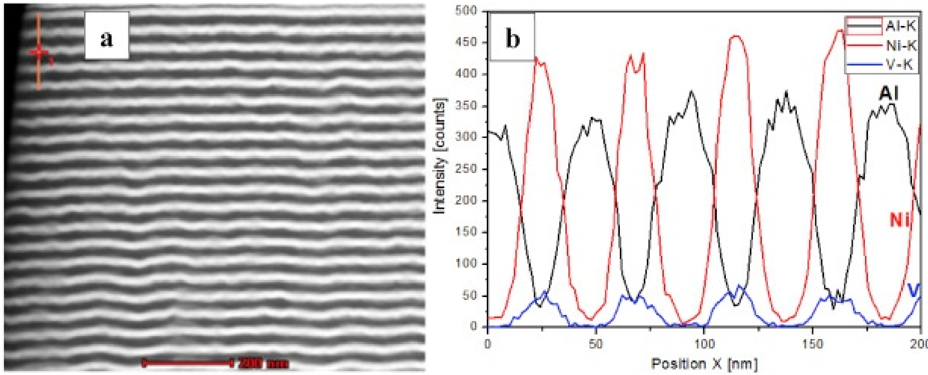
Applications for adiabatic calculations: hot topping

Thermo-Calc Software

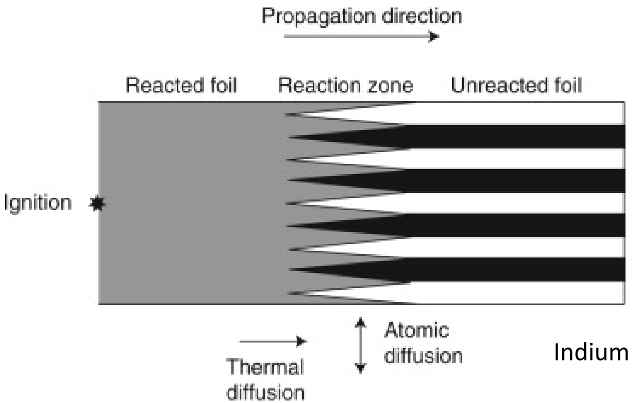
Exothermal mould powders at end of cast for continuous casting or for hot topping during ingot casting:
SiO_2 + CaO + FeO + xxx
+ Fe, Al, Si powder or …
→ Tuned energy release triggered by heat of Liquid steel

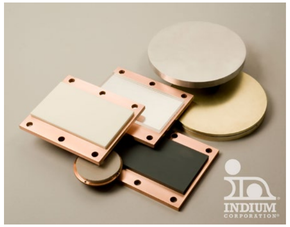
Applications for adiabatic calculations:

Nanofoil® for bonding, Self-healing multilayers, nano-heaters, dot heaters…

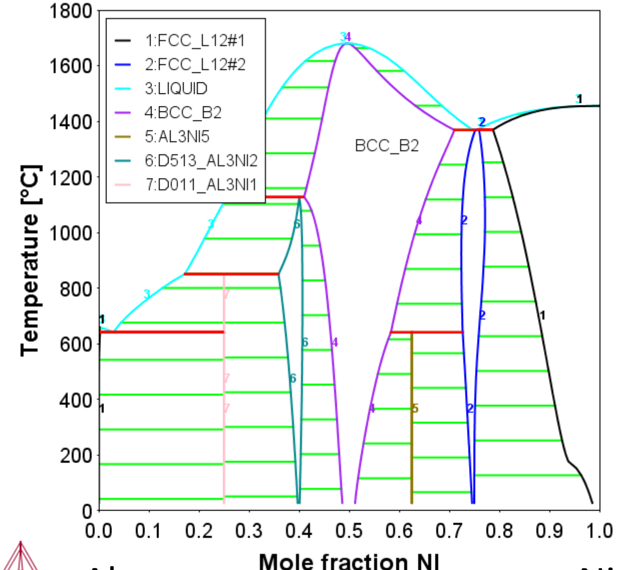


Łukasz Maja, Jerzy Morgiela, Maciej Szlezyngera, Piotr Bałab, Grzegorz Ciosb, Mat. Chem. Phys. Volume 193, 2017, Pages 244-252





Indium corporation: www.indium.com



Al Ni

Al + Ni → AlNi BCC_B2

→ Adiabatic calculation for T increase

→ Diffusion calculation for kinetics

THE WORLD COMES HERE TMS2020 149th Annual Meeting & Exhibition
CO-LOCATED INTERNATIONAL CONFERENCE PbZn 2020
February 23-27, 2020 San Diego, California, USA #TMSAnnualMeeting

Thermo-Calc Software

Applications for adiabatic calculations:

Heat patches for back-ache

Reaction:

Fe or FeO (powder) + O_2(gas)

→ FeO, Fe_3O_4, Fe_2O_3

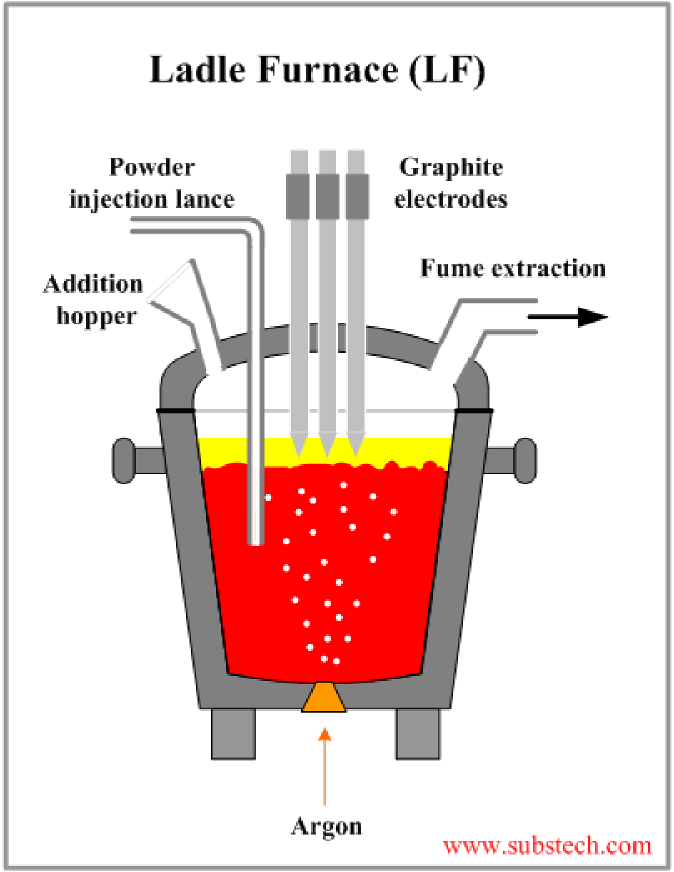
Thermo-Calc Software

)

Modelling of steel making / refining with TCOX9

- ❑ Simulation of secondary steel making (Ladle Furnace)
- ❑ Present in every steel-plant
- ❑ Comparison with scientific study from M.-A. van Ende et al. (2017)
- ❑ Actual experimental data from K. J. Graham et al. (2009)

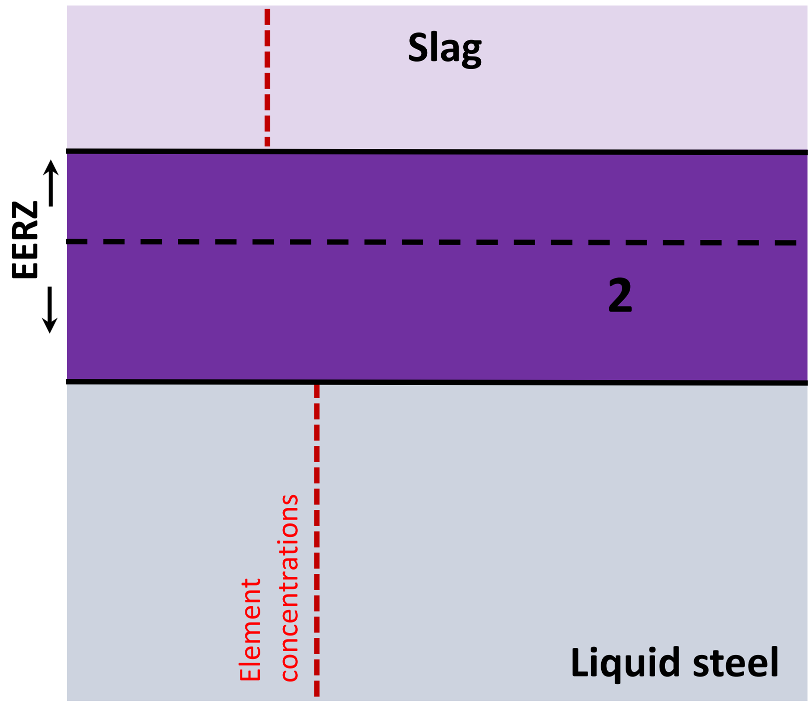
→**Kinetic model needed!**



Kinetic modelling of steelmaking with TCOX9

Thermo-Calc Software

Kinetic modelling using the **E**ffective **E**quilibrium **R**eaction **Z**one

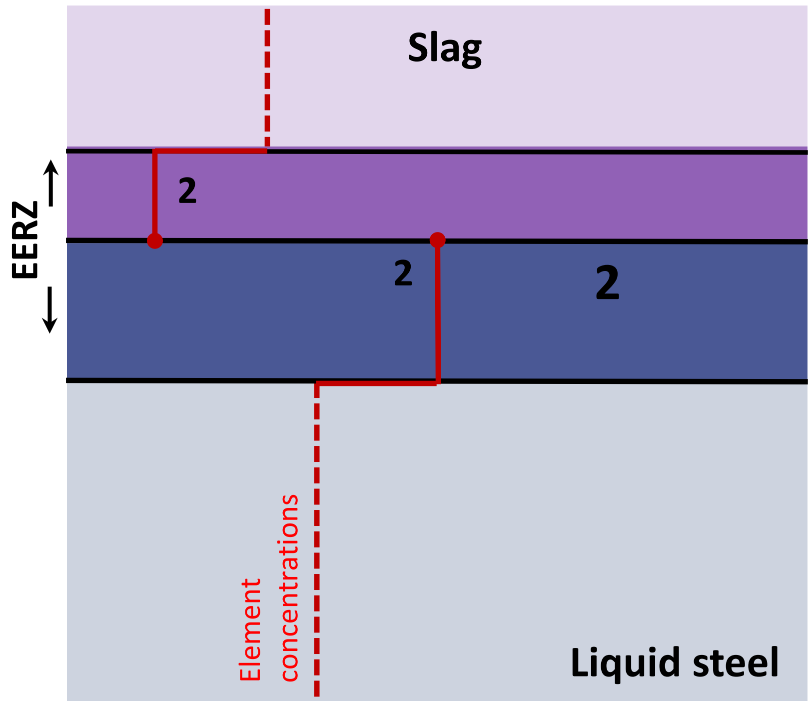


1. Transport to the reaction zone
2. Equilibrium within the EERZ

Kinetic modelling of steelmaking with TCOX9

Thermo-Calc Software

Kinetic modelling using the **E**ffective **E**quilibrium **R**eaction **Z**one

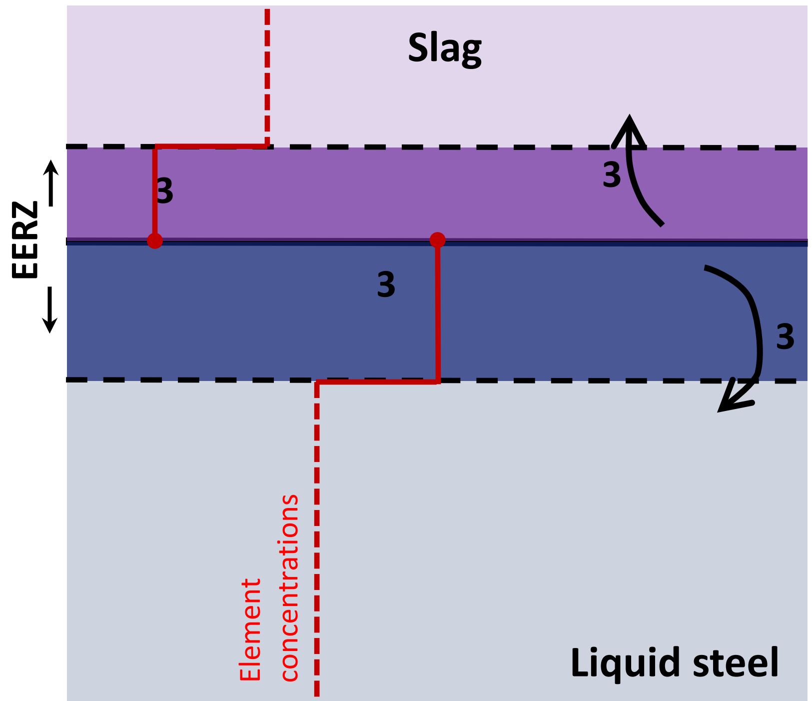


1. Transport to the reaction zone
2. Equilibrium within the EERZ

Equilibrium steel-slag inferface

Kinetic modelling of steelmaking with TCOX9

Kinetic modelling using the **E**ffective **E**quilibrium **R**eaction **Z**one

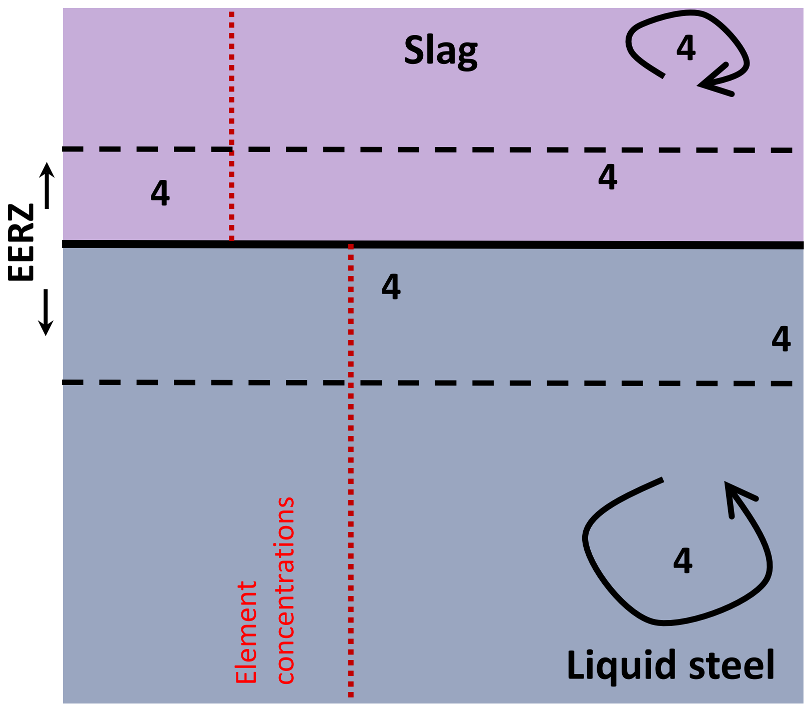


1. Transport to the reaction zone
2. Equilibrium within the EERZ,
3. Transport away from the EERZ

TMS 2020 149th Annual Meeting & Exhibition; LMPC 2019 Liquid Metal Processing & Casting Conference 2019; PbZn 2020; February 23-27, 2020 San Diego, California, USA #TMSAnnualMeeting

Kinetic modelling of steelmaking with TCOX9

Kinetic modelling using the **E**ffective **E**quilibrium **R**eaction **Z**one



1. Transport to the reaction zone
2. Equilibrium within the EERZ,
3. Transport away from the EERZ
4. Mixing in the bulk slag / liquid steel

References

J. Peter, K.D. Peaslee, D.G.C. Robertson, and B.G. Thomas, Proc. AISTech, 2005, vol. 1, pp. 959 – 73

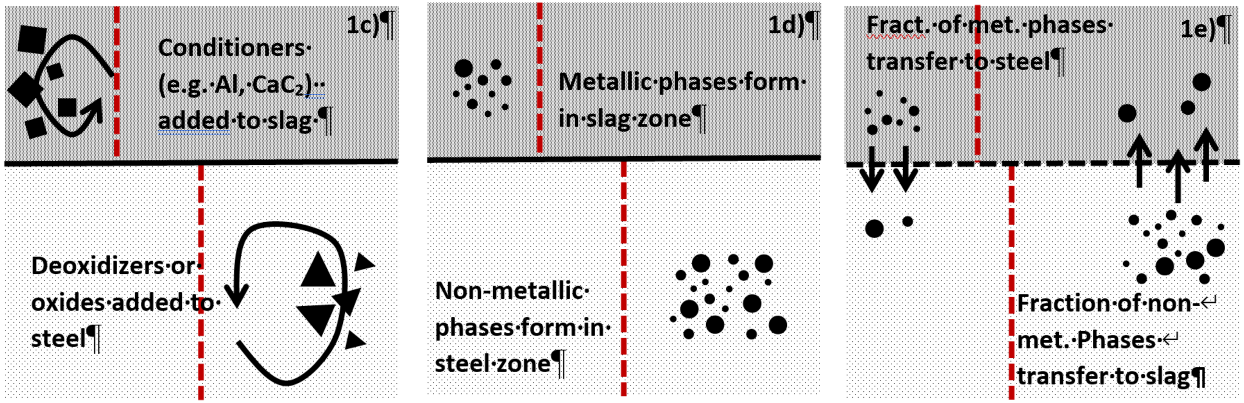
A. Harada, N. Maruoka, H. Shibata, and S. Kitamura, ISIJ Int., 2013, vol. 53, pp. 2110 - 2117

M.-A. van Ende and I.-H. Jung, Met. Mat Trans. B, 2017, Vol 48B, pp. 28 - 36

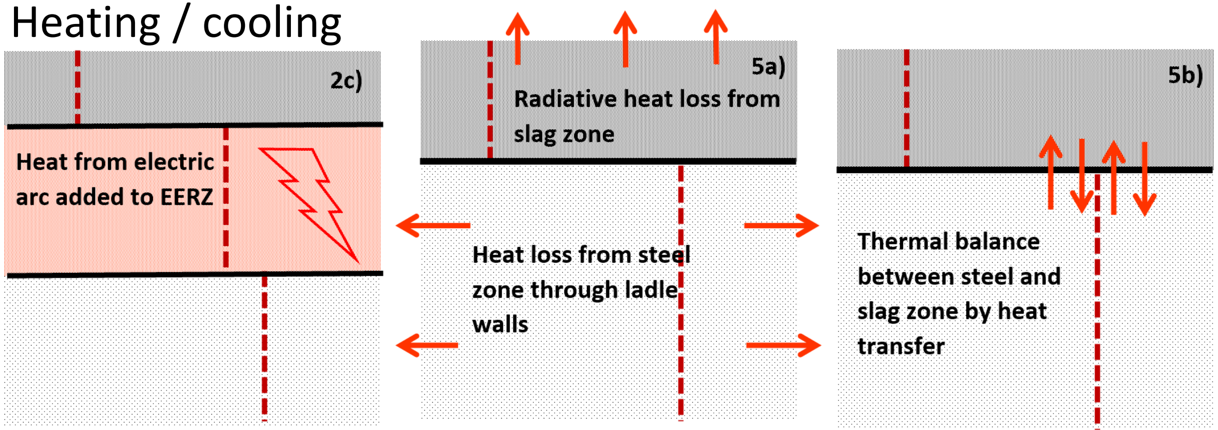
Kinetic modelling of steelmaking with TCOX9

Thermo-Calc Software

Inclusion formation and flotation / modification



Heating / cooling



THE WORLD COMES HERE
TMS2020
149th Annual Meeting & Exhibition
CO-LOCATED INTERNATIONAL CONFERENCE
PbZn 2020
February 23-27, 2020
San Diego, California, USA
#TMSAnnualMeeting

Kinetic modelling of steelmaking with TCOX9

AIST Transactions

Vol. 6, No. 1

Toward Integrated Ladle Metallurgy Control

K.J. Graham (formerly of McMaster University), Materials Institu… (kevin_graham@mckinsey.com), and **G.A. Irons,** Steel Research C… McMaster University, Hamilton, Ont., Canada (ironsga@mcmaste…

INTRODUCTION

During the last 50–60 years, considerable interest has been focused on the kinetics of sulfur removal from iron and steel.[1–8] Key findings from these kinetic studies have demonstrated that sulfur transfer from metal

kinet… simul… react… appli… descr…

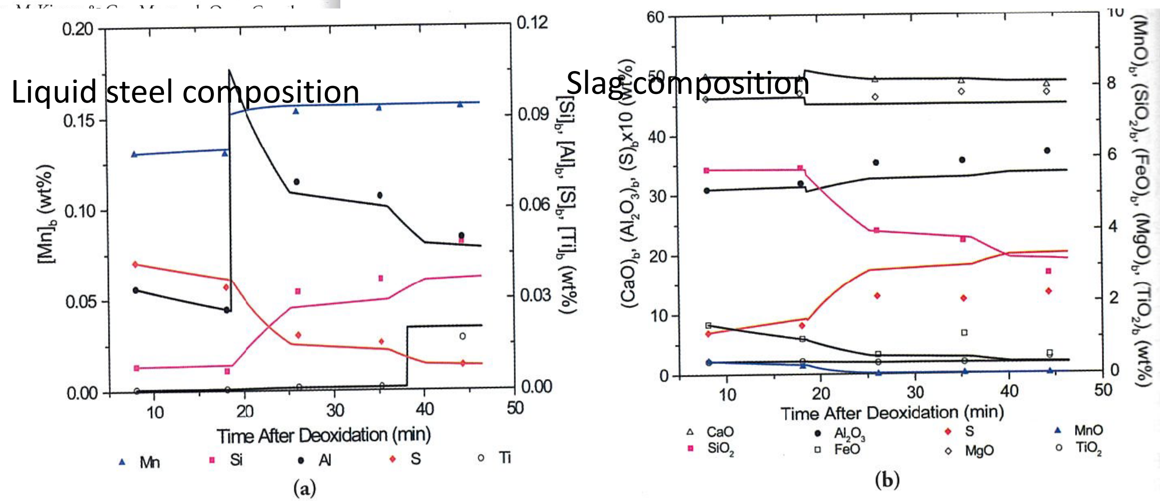


Figure 9
Comparison of experimental and model predicted results for: (a) $[wt\%S]_b$, $[wt\%Mn]_b$, $[wt\%Al]_b$, $[wt\%Si]_b$ and $[wt\%Ti]_b$, and (b) $(wt\%S)_b$, $(wt\%CaO)_b$, $(wt\%Al_2O_3)_b$, $(wt\%MnO)_b$, $(wt\%SiO_2)$, $(wt\%FeO)_b$, $(wt\%MgO)_b$ and $(wt\%TiO_2)$.

Ladle Furnace Refining

Initial steel: 165 t, 1600°C

Fe-0.12 Mn-0.008 Si-0.001 Al-0.001Ti-0.06 S-0.01 O

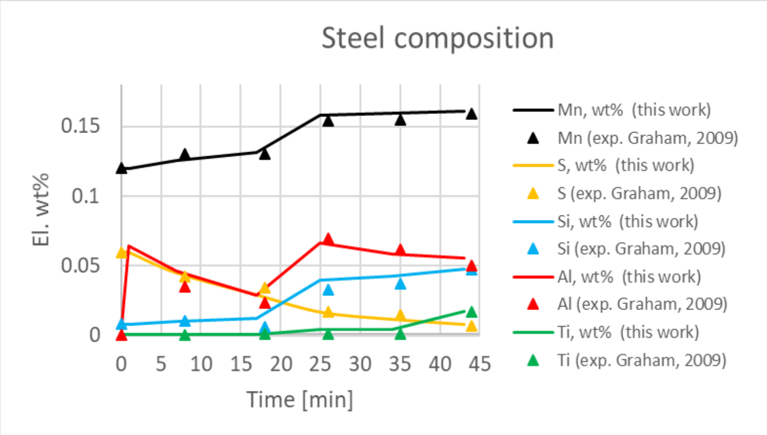
Initial slag: 4.95 t, 1600°C

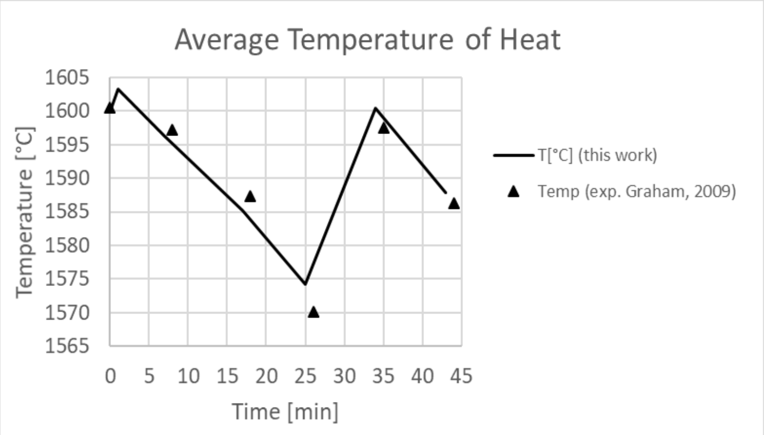
50 CaO-31.2 Al_2O_3-8 MgO-6.0 SiO_2-0.8 MnO-1.9 FeO-2.19 TiO_2-0.01 S

Process parameters:

At tap: Al killing with 105 kg Al
20 min: 100 kg CaO, 140 kg Al, 50 kg FeMn added
27 min-34 min: Electric arc heating
39 min: 46 kg FeTi added

→ Manual simulation with 6 calculation steps in console mode





Ladle Furnace Refining

Thermo-Calc Software

Initial steel: 165 t, 1600°C

Fe-0.12 Mn-0.008 Si-0.001 Al-0.001Ti-0.06 S-0.01 O

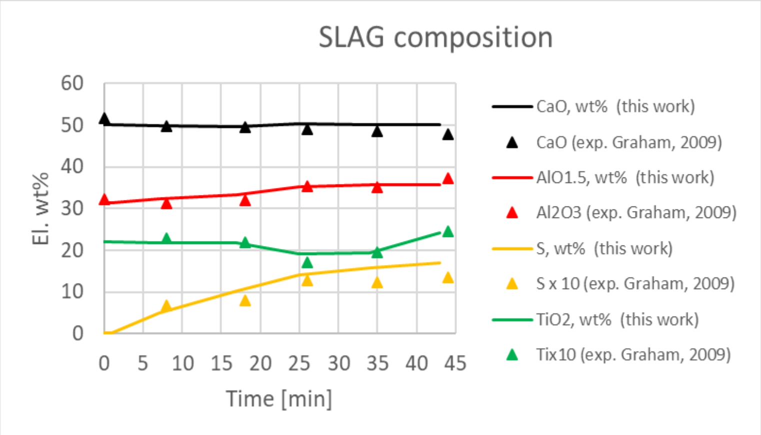
Initial slag: 4.95 t, 1600°C

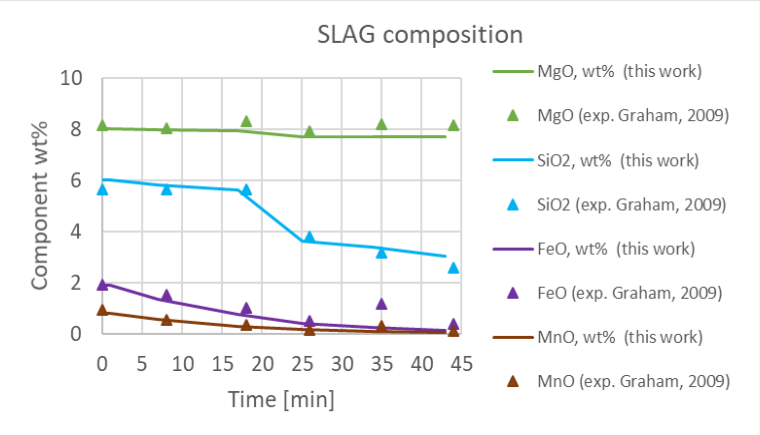
50 CaO-31.2 Al_2O_3-8 MgO-6.0 SiO_2-0.8 MnO-1.9 FeO-2.19 TiO_2-0.01 S

Process parameters:

At tap: Al killing with 105 kg Al
20 min: 100 kg CaO, 140 kg Al, 50 kg FeMn added
27 min-34 min: Electric arc heating
39 min: 46 kg FeTi added

→ Manual simulation with 6 calculation steps in console mode





Ladle Furnace Refining

Initial steel: 165 t, 1600°C

Fe-0.12 Mn-0.008 Si-0.001 Al-0.001Ti-0.06 S-0.01 O

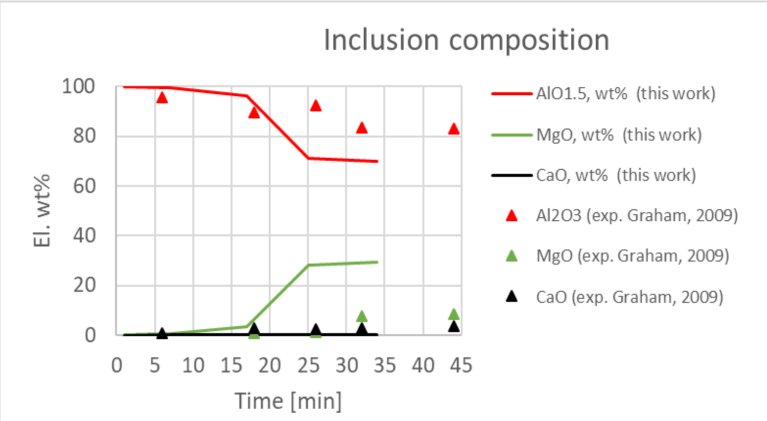
Initial slag: 4.95 t, 1600°C

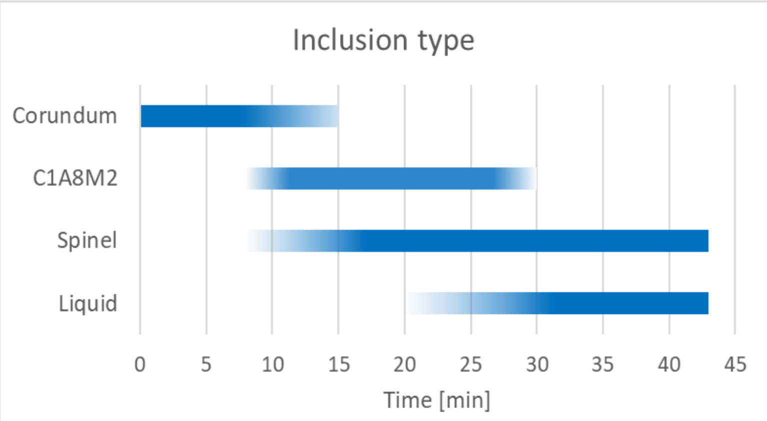
50 CaO-31.2 Al_2O_3-8 MgO-6.0 SiO_2-0.8 MnO-1.9 FeO-2.19 TiO_2-0.01 S

Process parameters:

At tap:	Al killing with 105 kg Al
20 min:	100 kg CaO, 140 kg Al, 50 kg FeMn added
27 min-34 min:	Electric arc heating
39 min:	46 kg FeTi added

→ Manual simulation with 6 calculation steps in console mode





Python calculation set-up

Thermo-Calc Software

Model configuration, kinetic parameters

```python
# model configuration
database = "TCOX10"
pressure_in_pa = 1.0e5
diameter = 5.0  # in m
delta_time = 60.0  # in s
time_end = 45 * 60  # in s
heat_loss_steel = -3.583e6  # in W
heat_transfer_coeff_steel_and_slag = 5.0e3  # in W/(m**2 * K)
inclusion_removal_rate = 4.5  # in %/min
heat_electric_arc = 11.657e6  # in W
electric_arc_heating_times = {"min":27,"max":34}# in min
steel_mass_transfer_coeff = 0.00089779711487773584  # in m/s
steel_density = 7800  # in kg/m**3
slag_mass_transfer_coeff = 4.6685449973622263e-05  # in m/s
slag_density = 4500  # in kg/m**3
low_stirring_gas_flow = 0.167 / 60  # in Nm**3/s
high_stirring_gas_flow = 0.5 / 60  # in Nm**3/s
area = (diameter / 2)**2 * np.pi
```

Materials compositions

```python
with TCPython(debug_mode=True) as session:
    steel = Material(Composition.relative_composition(
        {"Fe":None,"Mn":0.12,"Si":0.008,"Al":0.001,"Ti":0.001,"S":0.06,"O":0.01,"C":0.04},
        RelativeUnit.WEIGHT_PERCENT),165,AbsoluteUnit.TONNE,temperature_in_k=1600 + 273.15)

    oxygen_comp = Composition.relative_gas_composition({"O2":100})

    slag = Material(Composition.relative_composition(
        {"CaO":50,"Al2O3":31.1,"MgO":8,"SiO2":6,"MnO":0.8,"FeO":1.9,"TiO2":2.19,"S":0.01},
        RelativeUnit.WEIGHT_PERCENT),4.95,AbsoluteUnit.TONNE,temperature_in_k=1600 + 273.15)
```

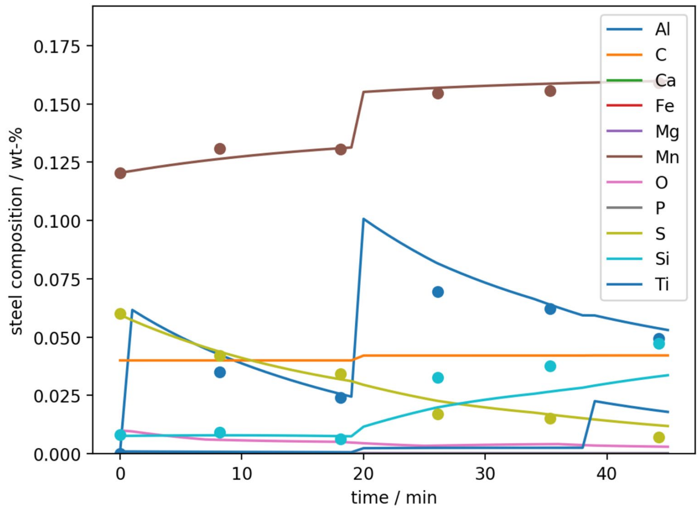
Time stepping / material addition amounts and times

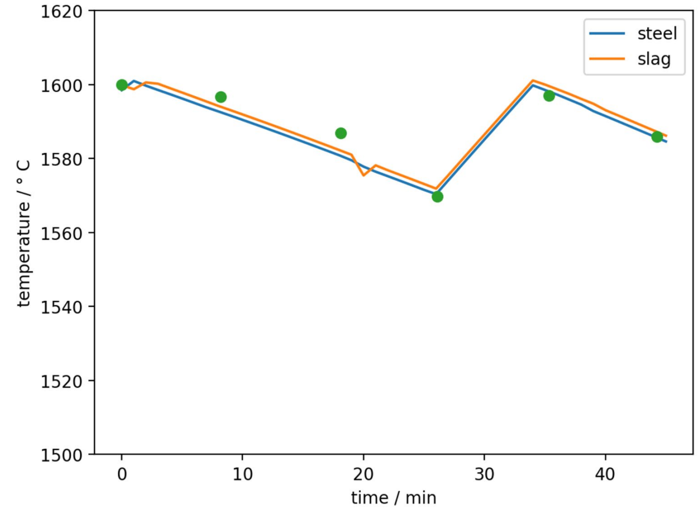
```python
# energy transfer
calc.add_power_to_zone("steel",heat_loss_steel)
calc.add_power_to_reaction_zone("steel","slag",heat_electric_arc,60 * electric_arc_heating_times["min"],
                               60 * electric_arc_heating_times["max"]+ delta_time)
times = np.arange(0,time_end + delta_time,delta_time)
for sim_time in times:
    # material additions
    if len(additions) > 0:
        indices_to_remove = []
        for addition_index,addition in enumerate(additions):
            if sim_time / 60 >= addition["time_in_min"]:
                if addition["zone"]== "reaction_zone":
                    calc.add_material_to_reaction_zone_at_time("steel","slag",addition["material"],sim_time)
                else:
                    calc.add_material_to_zone_at_time(addition["zone"],addition["material"],sim_time)
                indices_to_remove.append(addition_index)
        for index in sorted(indices_to_remove,reverse=True):
            del additions[index]
result = calc.calculate()
times = np.array(result.get_times())
```

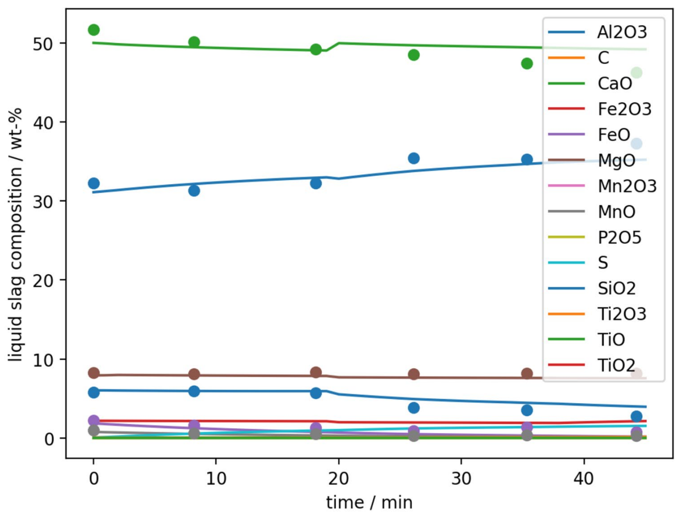
→ Calculate (app. 10 min)

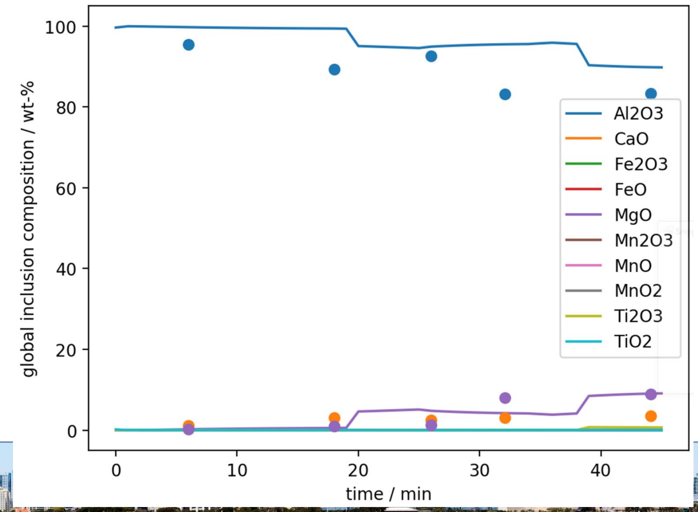
→ Plot

Python calculation results



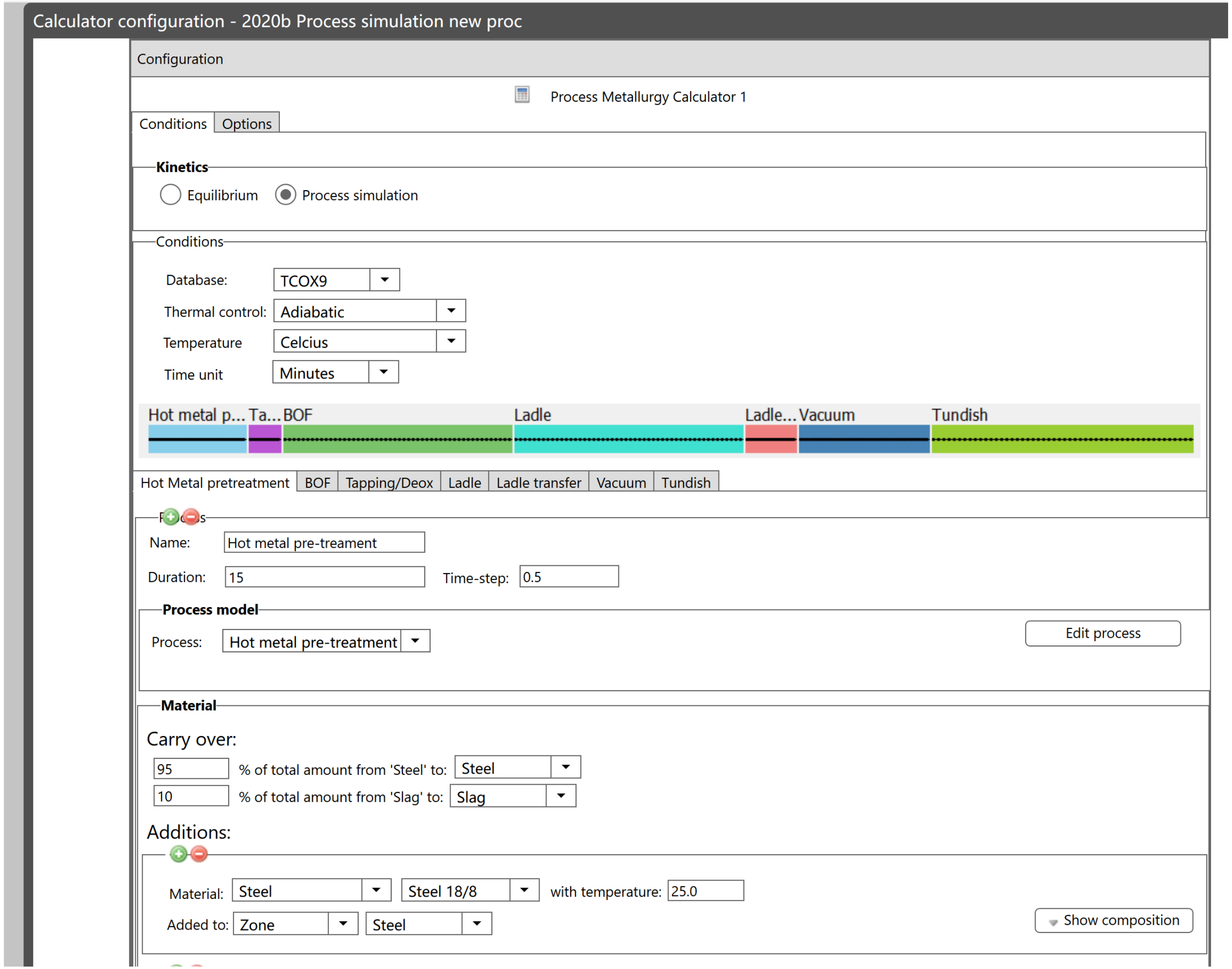






Release of Thermo-Calc's Process Metallurgy Module!

Thermo-Calc Software



Link processing steps

→ Digital Twin of process

Thank you!

Contact: nicholas@thermocalc.com

…and please visit our booth