A model for the prediction of precipitate formation during steel making

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Contents

- Introduction
- Description of the model for the prediction of inclusion composition
- What is SimuSage?
- Thermodynamic and kinetic factors
- Model validation in the industrial processes (210t and 30t melts)
- Assistance in the industrial process
- Conclusions

Contents

- ***Why?***

Why was this simulation model made?

- ***How?***

How was it done?

- ***What?***

What kind of results does it give?

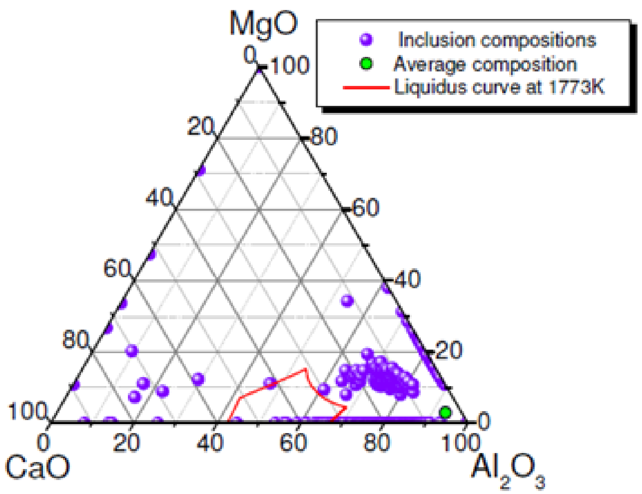
- **Steel cleanliness is a major issue**
- **Ever increasing requirement for strict control of inclusion composition and amount during ladle treatment**

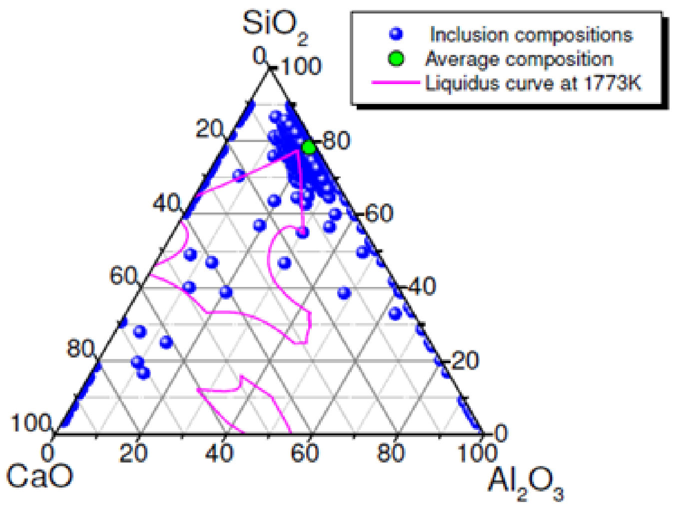
- **Tasks in ladle metallurgy:**
  - Adjustment of chemical composition
  - Adjustment of temperature
  - Separation of inclusions
  - …

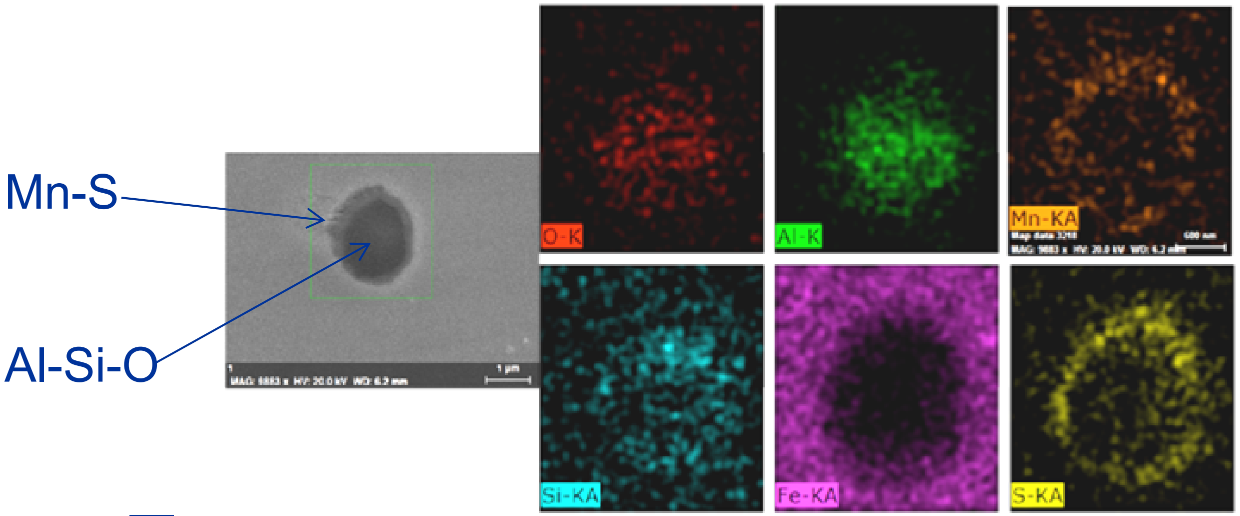
Intention:

to develop a robust model predicting the inclusion composition and amount which can be used on-line in the industrial process (using a PC)

Inclusion compositions at early stage of LF refining

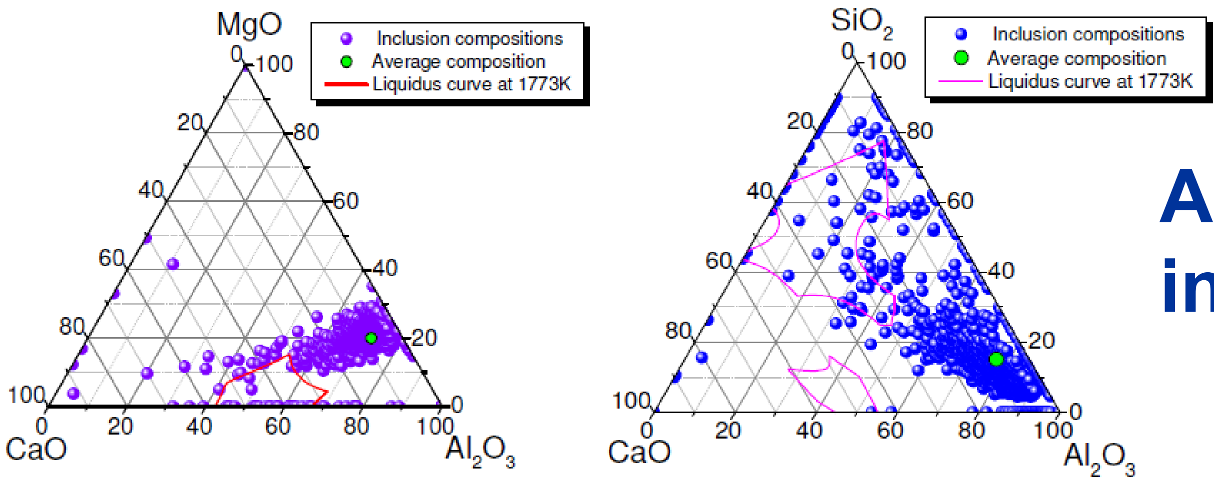






Zhang, Proc. VDEh-CSM Seminar, Düsseldorf, 2014

After alloying in LF



. Inclusion compositions after alloying during LF refining

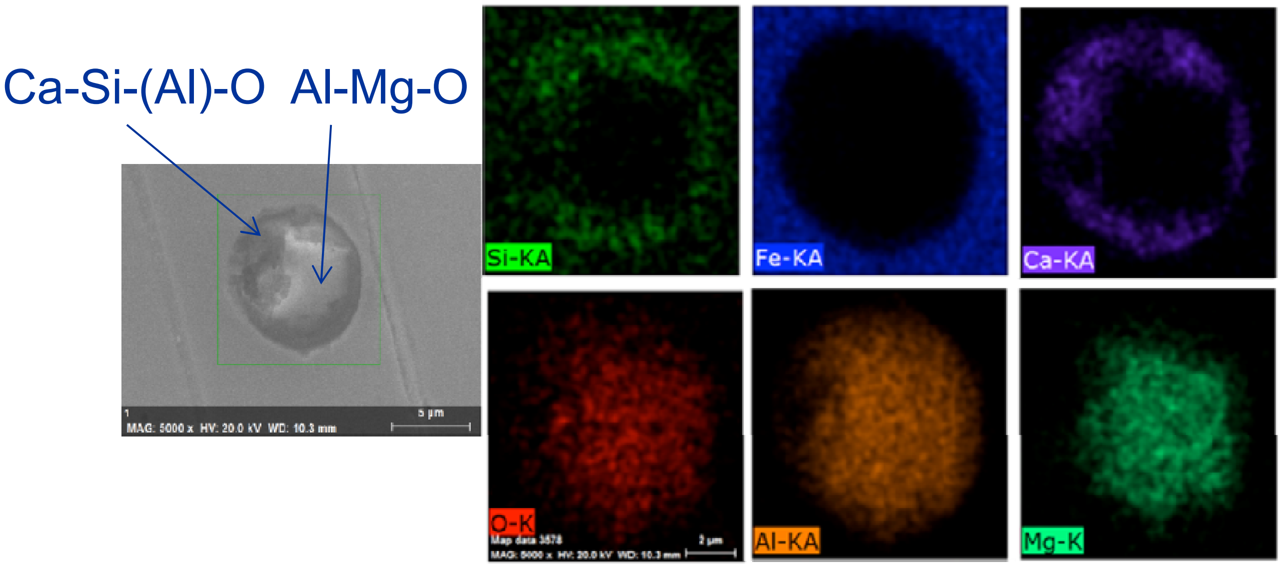
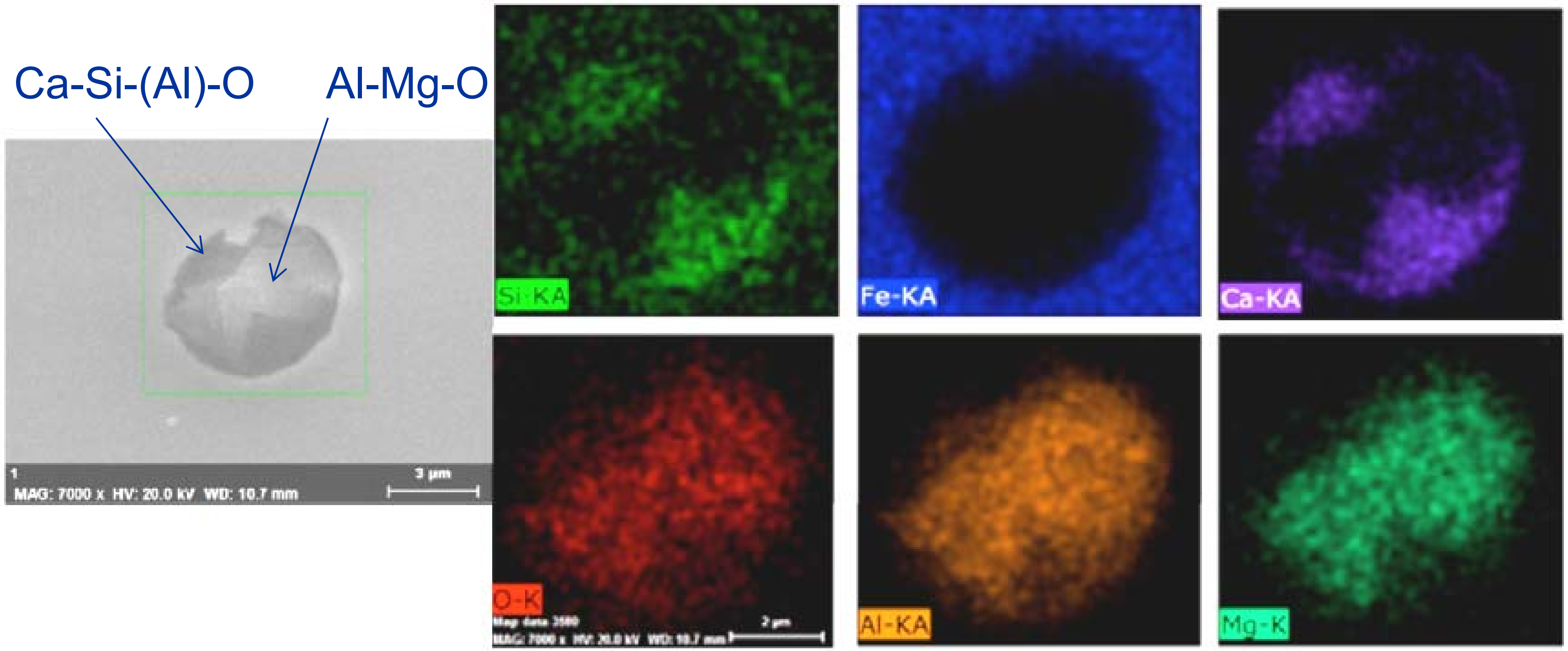


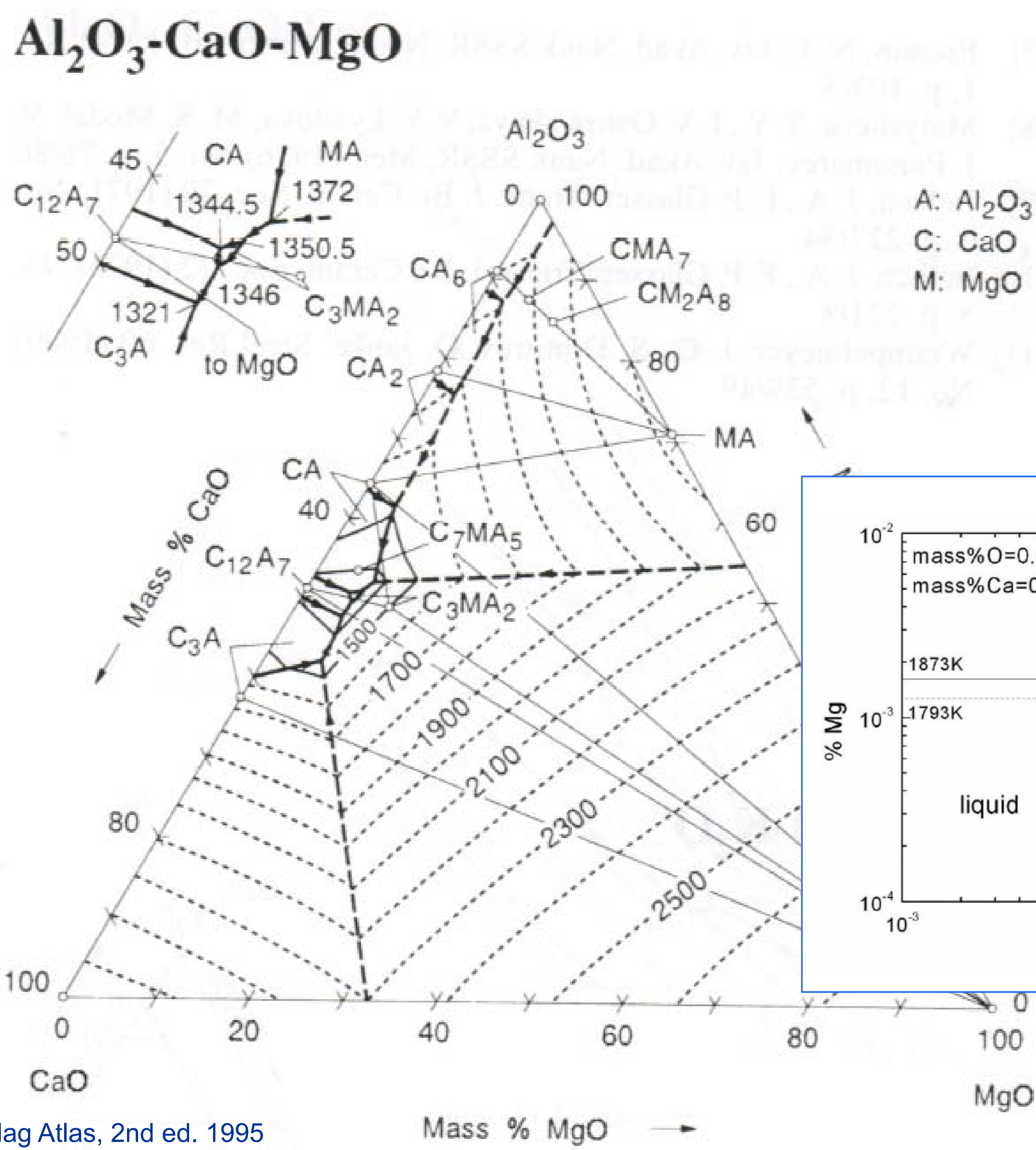
Figure 4. Elemental mappings of a typical inclusion after alloying during LF refining

Zhang, Proc. VDEh-CSM Seminar, Düsseldorf, 2014

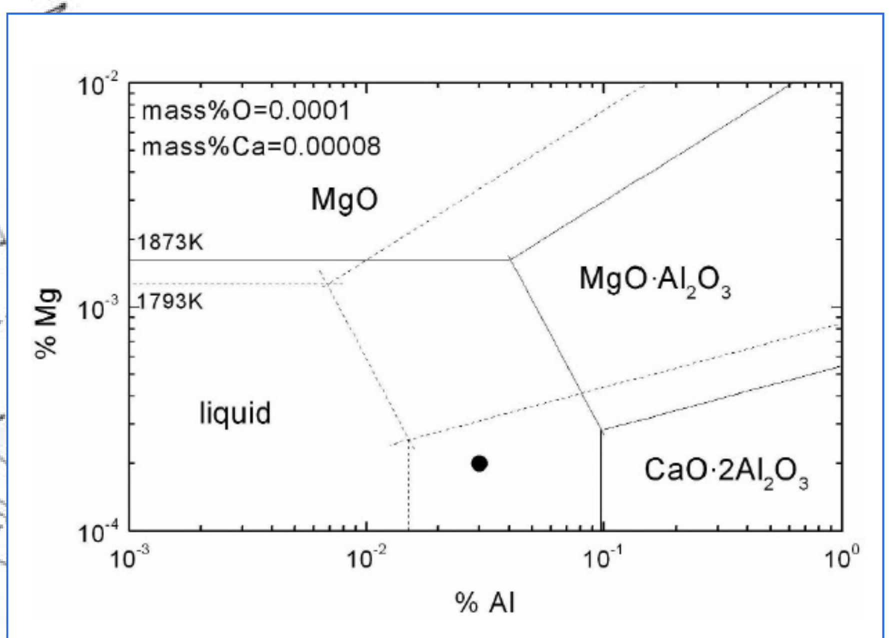
Typical inclusion before vacuum refining



Elemental mappings of a typical inclusion before vacuum refining



Stability diagram of Fe-Al-Mg-Ca system at 1873K and 1793K.



~~Kang et al., steel res. int. 77 (2006) 11, 78~~

Slag Atlas, 2nd ed. 1995

Non-metallic inclusions during the process

Inclusion composition

$$f = (a_{i=1\text{ to }x,\text{ including soluble Oxygen}},\ T,\ p)$$

Activity of all species changes continuously because of:

- Reactions metal-slag
- Reactions metal refractory
- Reactions slag-refractory
- Separation of inclusions to slag
- Temperature change

Result:

Continuous change of inclusion composition!

Inclusion origin, composition and heterogeneity

Origin

- Exogenous (not in the model)
- Endogenous
  - Product of reactions between phases
  - Product of local changes in phase equilibria

Composition

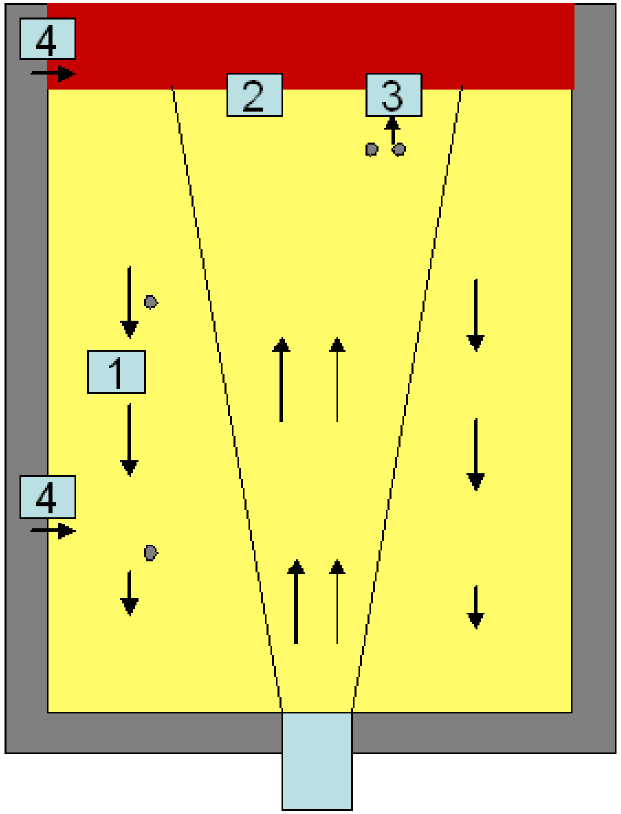
- Depending on local phase equilibria
- Depending on reactions at phase interfaces

Heterogeneity

- Nuclei surrounded by later precipitated phase
- Agglomeration
- Disintegration of homogeneous phase because of
  - local change of species activities
  - temperature drop

Model Description

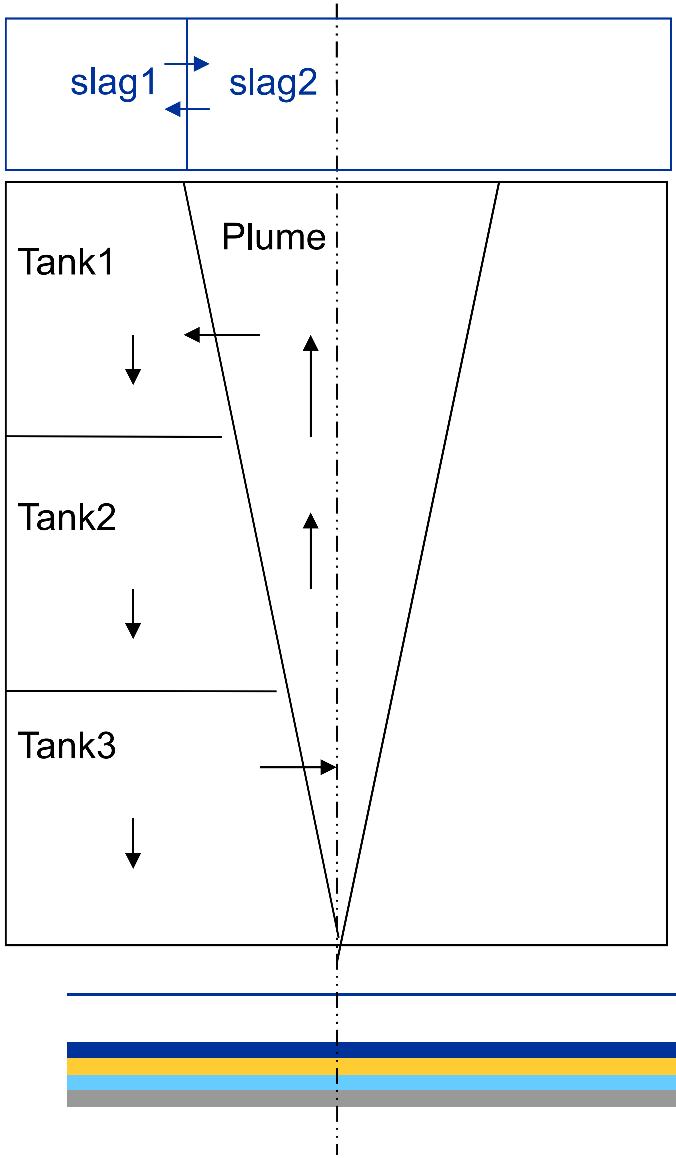
Reaction sites and parameters implemented in the Model



1: Mixing in the ladle
2: Slag-Metal reaction
3: Inclusion separation
4: Lining interaction with steel and slag

Model Description

The mixing in gas stirred ladle



- Tank1,2,3 with same height
- Diameter of plume is set as ½ of ladle diameter (related to medium Ar-flow rate)
- Tracer concentration (e.g. of transferred mass of species *i*) in tank N at time t:

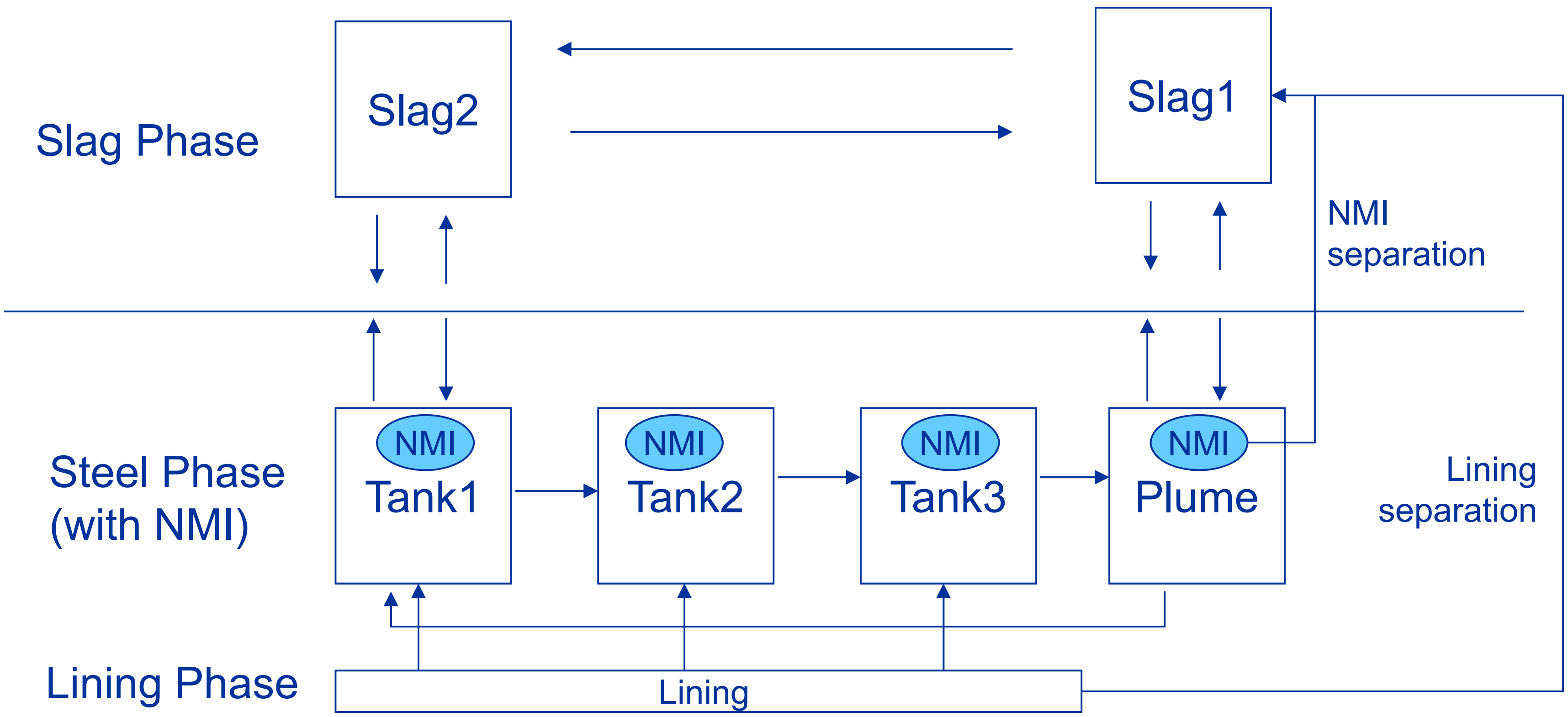
$$C(N,t) = \frac{C(N,t-\Delta t)(M(N)-r_M\Delta t)+C(N-1,t-\Delta t)(r_M\Delta t)}{M(N)}$$

where
C(N,t) are concentration in tank N at time t,
M(N) is the mass of tank N and
r_M is the mass recirculation rate (obtained from industrial trials).

The phase equilibria calculation follows the mass flow and is calculated for each tank every 5 seconds.

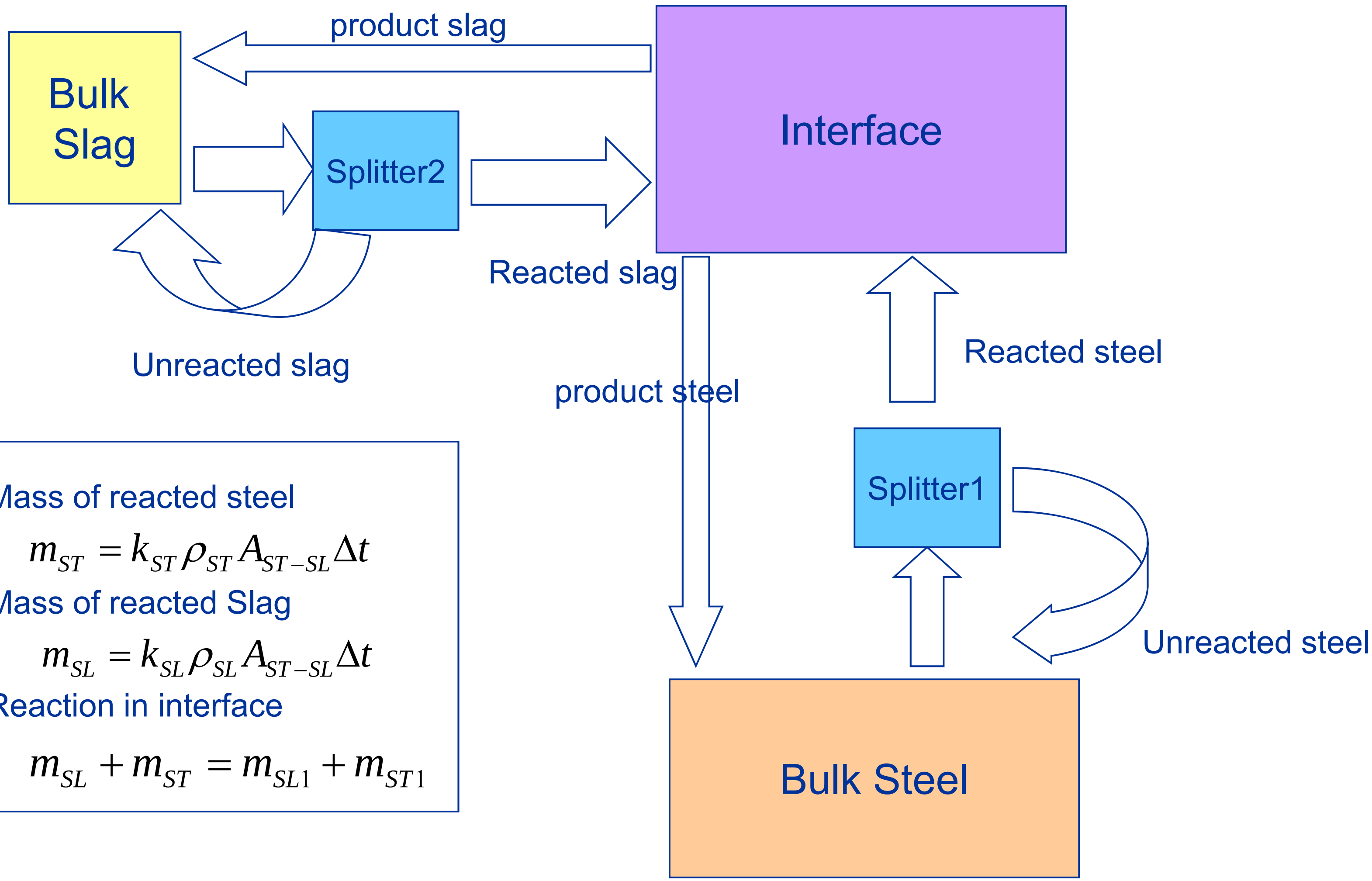
Model Description

Schema of the model



Model Description

Schema for slag-metal reaction



Mass of reacted steel

$$m_{ST} = k_{ST}\rho_{ST}A_{ST-SL}\Delta t$$

Mass of reacted Slag

$$m_{SL} = k_{SL}\rho_{SL}A_{ST-SL}\Delta t$$

Reaction in interface

$$m_{SL} + m_{ST} = m_{SL1} + m_{ST1}$$

Model Description

Local thermodynamic equilbiria

- Thermodynamic equilibrium between steel and inclusions in each tank
- Thermodynamic equilibrium between slag and steel at the slag-steel interface
- Thermodynamic equilibrium between steel and dissolved lining material

Kinetic parameters

- **Based on measurements in the industrial process:**

  fluid dynamic, mixing, mass transfer coefficients, lining dissolution, separation of NMI (separation rate depending on nature of inclusions and process development)

Model Description

Model tools

SimuSage

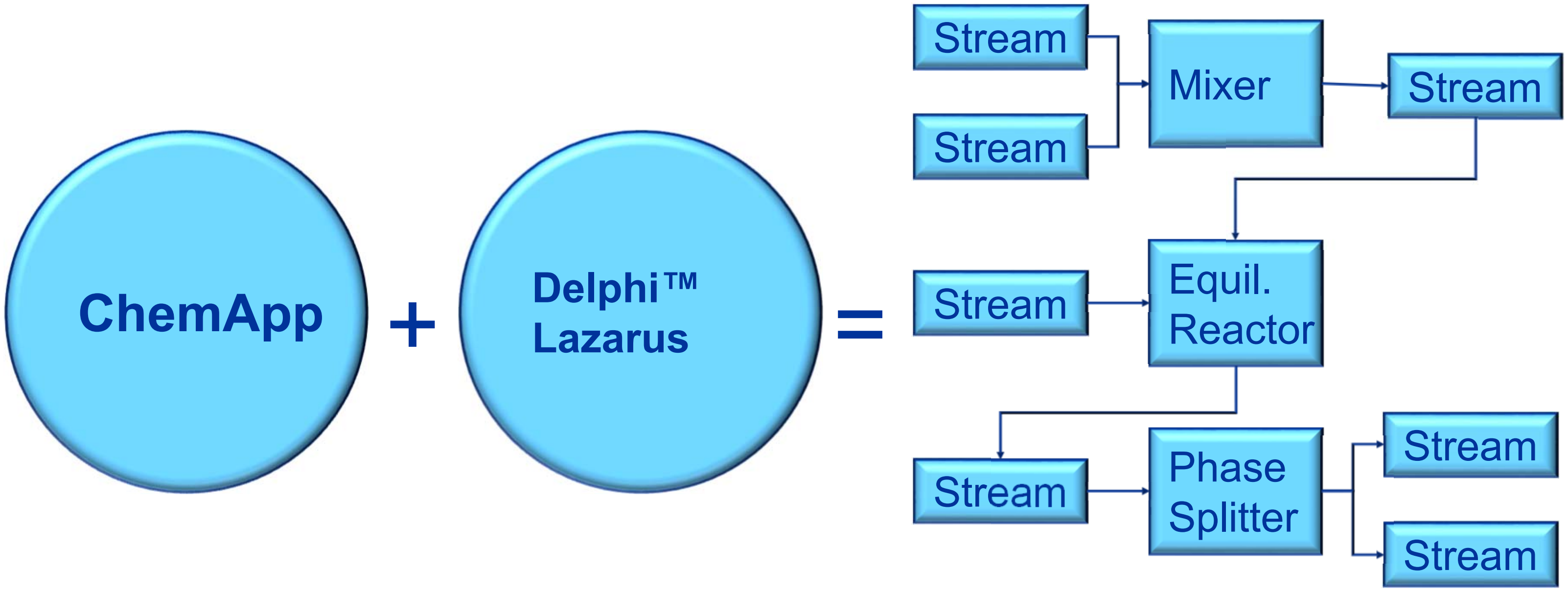
Various basic unit operation components in SimuSage used:

- equilibrium reactor
- mixer
- splitter
- iterator …

FactSage: source for thermodynamic data of various phases (steel, slag, inclusions, lining refractory)

What is SimuSage?

- SimuSage is a ChemApp-based set of Delphi/Lazarus components for process simulation (flowsheeting) tasks



SimuSage ...

- ... is a toolkit for Delphi™
  - Win32 development
  - 100% embedded in Delphi
  - All Delphi programming features can be used
  - Creates Win32 executables
  - Available for Delphi 6, 7, 2005, 2006, 2007, 2009, 2010, XE, XE2 ...

EMBARCADERO TECHNOLOGIES

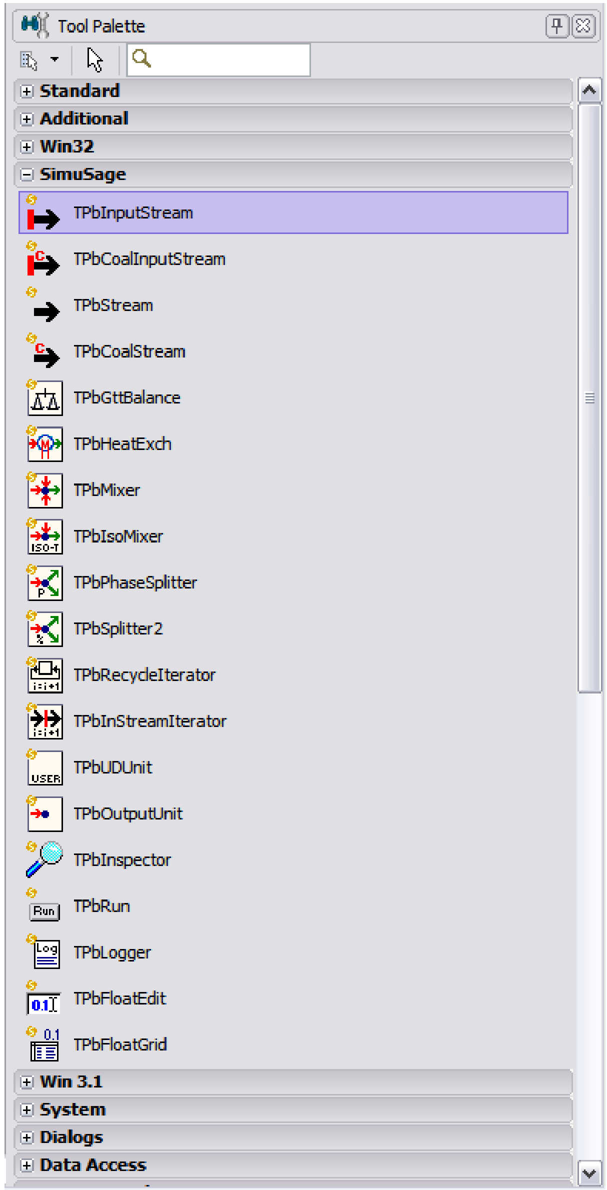
TECHNOLOGY PARTNER

- … is also available for Lazarus
  - Open Source „Delphi-compatible“ development environment
  - Based on Free Pascal
  - LGPL licensed libraries, GPL licensed IDE

Lazarus

SimuSage ...

- ... is a set of visual and non-visual components
  - Visual programming
  - RAD (Rapid Application Development)



The benefits (summary)

- RAD (Rapid Application Development) of process simulations/flowsheets with a minimum amount of programming.
- Virtually no restrictions as to the complexity of the simulation; dynamic as well as steady state
- Fully integrated into Delphi, all language features and programming tools available.
- Benefits of OO design: Reusability of components, extensibility through inheritance, etc.
- Visual programming, resulting in fast 32 bit Windows programs.
- Resulting programs can be distributed to end users, no Delphi required.
- Datafile for reusable stream and material definitions.

Overview on SimuSage and its applications

Basic

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SimuSage – the component library for rapid process modeling and its applications

Dedicated to Dr. Gunnar Eriksson on the occasion of his 65th birthday

SimuSage is an innovative software tool for process simulation and flowsheeting tasks. Based on ChemApp and its rigorous Gibbs energy minimizing technique, it provides a library of components for the development of highly customized process simulation models. The SimuSage concept is described, and a number of examples from typical application areas such as metallurgy, combustion technology, and other industrial high-temperature processes involving inorganic chemistry are introduced.

Keywords: Thermochemistry; Gibbs energy minimization; Process simulation; Flowsheeting; Computer aided process engineering

1. Introduction

early stage the Institut für Verfahrenstechnik at RWTH Aachen University (IVT) successfully tested it in a number of complex process simulation projects and developed interesting new modeling concepts based on the new package. This process simulation tool has subsequently been made commercially available by GTT-Technologies as the software package SimuSage.

2. Requirements and specifications

Although a large variety of software tools had already been available at the time development of SimuSage started, no single tool matched more than a few of the requirements as determined by the developers. The catalog of requirements for such a new software package included points listed below.

2.1 Data availability

S. Petersen et al., "SimuSage - the component library for rapid process modeling and its applications", Int. Journal of Mat. Res., vol. 98(10), 2007, pp. 946-953

SimuSage projects

- Metallurgy
  - LD Converter
  - EAF, slag recycling
- Combustion / power generation
  - Biomass fired power plant
  - Pressurized pulverized coal combustion (PPCC)
  - Coal gasification, syngas production (coal-to-liquid technology)
  - Ash formation and deposition mechanisms in coal fired boilers
  - OXYCOAL-AC process
- Cement clinker production
- Advanced metal halide lamp chemistry

Local thermodynamic equilbiria

- Thermodynamic equilibrium between steel and inclusions in each tank;
- Thermodynamic equilibrium between slag and steel at the slag-steel interface;
- Thermodynamic equilibrium between steel and dissolved lining material.

Kinetic parameters

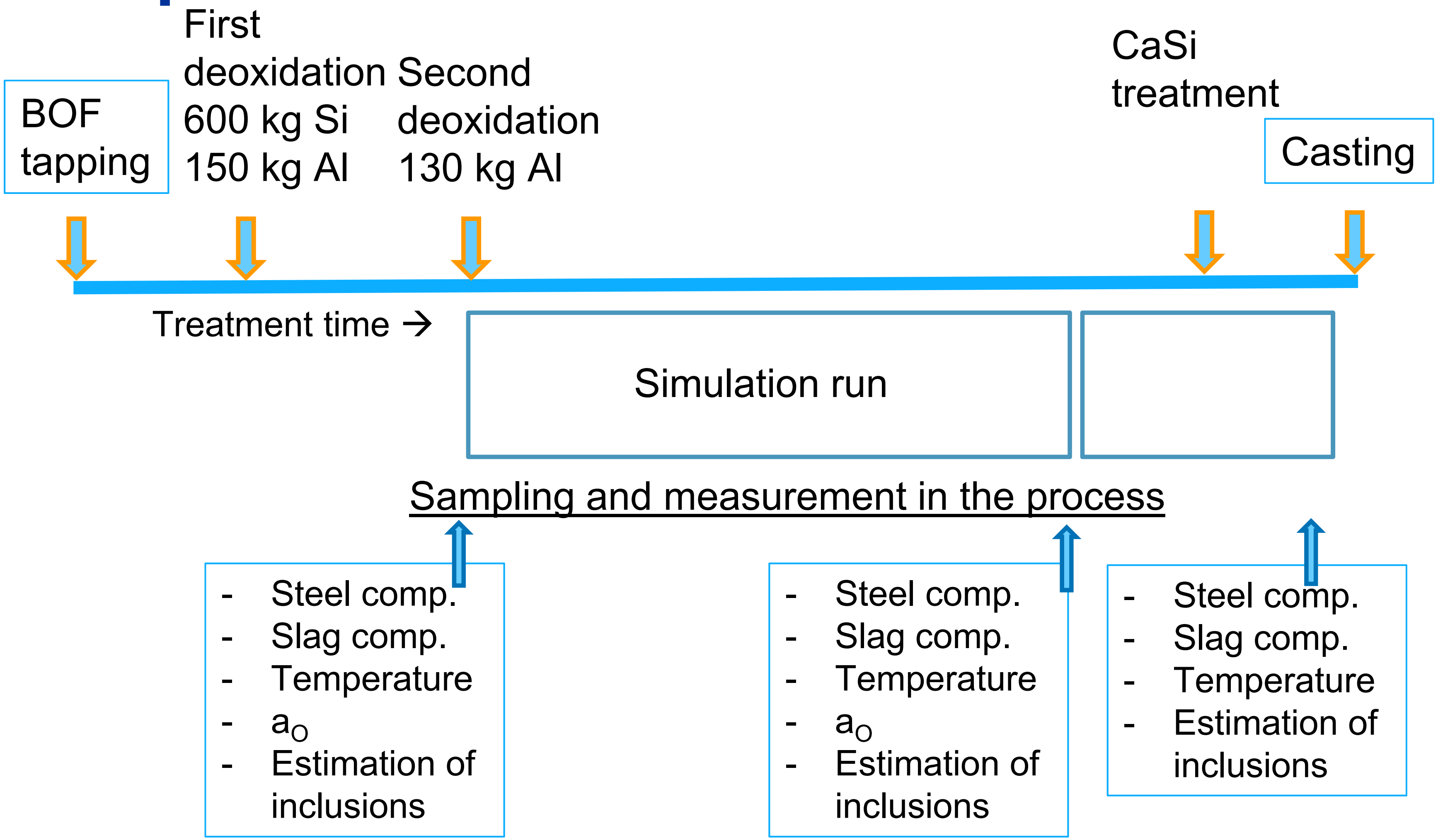
- **Based on measurements in the industrial process:**

fluid dynamic, mixing, mass transfer coefficients, lining dissolution, separation of NMI (separation rate depending on nature of inclusions and process development)

Model Validation

Validation in 210 t ladle, treatment of low alloyed steel

Model validation: Ladle treatment procedure for validated 210t heat



Model Validation

Industrial data for model validation

Steel and slag mass	Steel: 210000 kg, Slag: 2500 kg
Chemical composition of steel before treatment (starting values)	C: 0.11%; Mn: 0.90%; Cr: 0.24%; Mo: 0.12%; V: 0.007%;Ti: 0.002%
Chemical composition of slag before treatment (starting values)	CaO: 54%; SiO_2: 12%; Al_2O_3 :22%; MgO: 8%. CaF_2: 4%; FeO+MnO_2<<1% (after 2nd Al-addition)
Deoxidation regime	1) Si 600 kg Al 150kg 2) Al 130kg 3) CaSi treatment
Lining	MgO-C

Model Validation

Model parameters used for calculation

Recirculation rates (industrial data)	2800 kg/s (for medium Ar flow rate)
Mass transfer coefficients	Steel side: K_{ST}=0.002 m/s, Slag side: K_{SL}=0.001m/s.
Lining (MgO-C) dissolution rates (industrial data)	For contact with steel: 0.0005kg/(m^2.s) For contact with slag: 0.001kg/(m^2.s)
Bath temperature (derived from industrial trials)	Decrease with time (C.E. Grip, 77th Steelmaking conference proceedings 1994) $T = 1650 - 0.144t/60 - 8.689\sqrt{t/60}$

No adjustment or fitting of kinetic parameters in the simulation!

Separation of inclusion

industrial observation

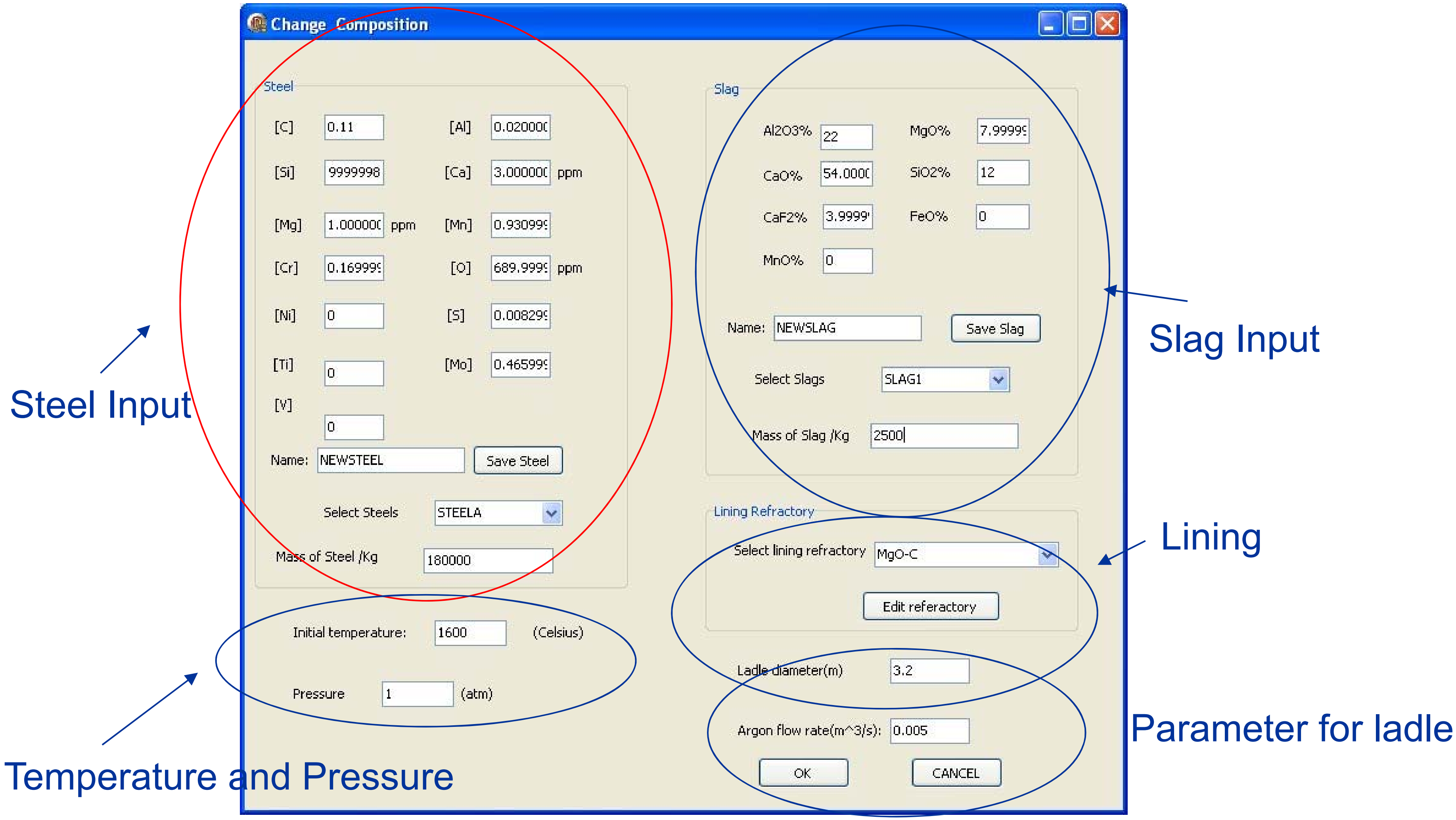
- Inclusions in plume tank separate into slag phase with different separation rates.
- Separation rates:

Inclusion type	Al_2O_3 and Al_2O_3 rich aluminates		Spinels	Liquid inclusions
Separation rates /per calculation time step(5s)	<10min	>10min	3%	5%
	20%	5%		

Input data

- Steel
  - Steel mass
  - Steel composition
- Slag
  - Slag mass
  - Slag composition
- Refractory
  - Type
  - Composition
- Initial temperature and pressure
- Ladle geometry
  - Ladle diameter
- Argon flow rates

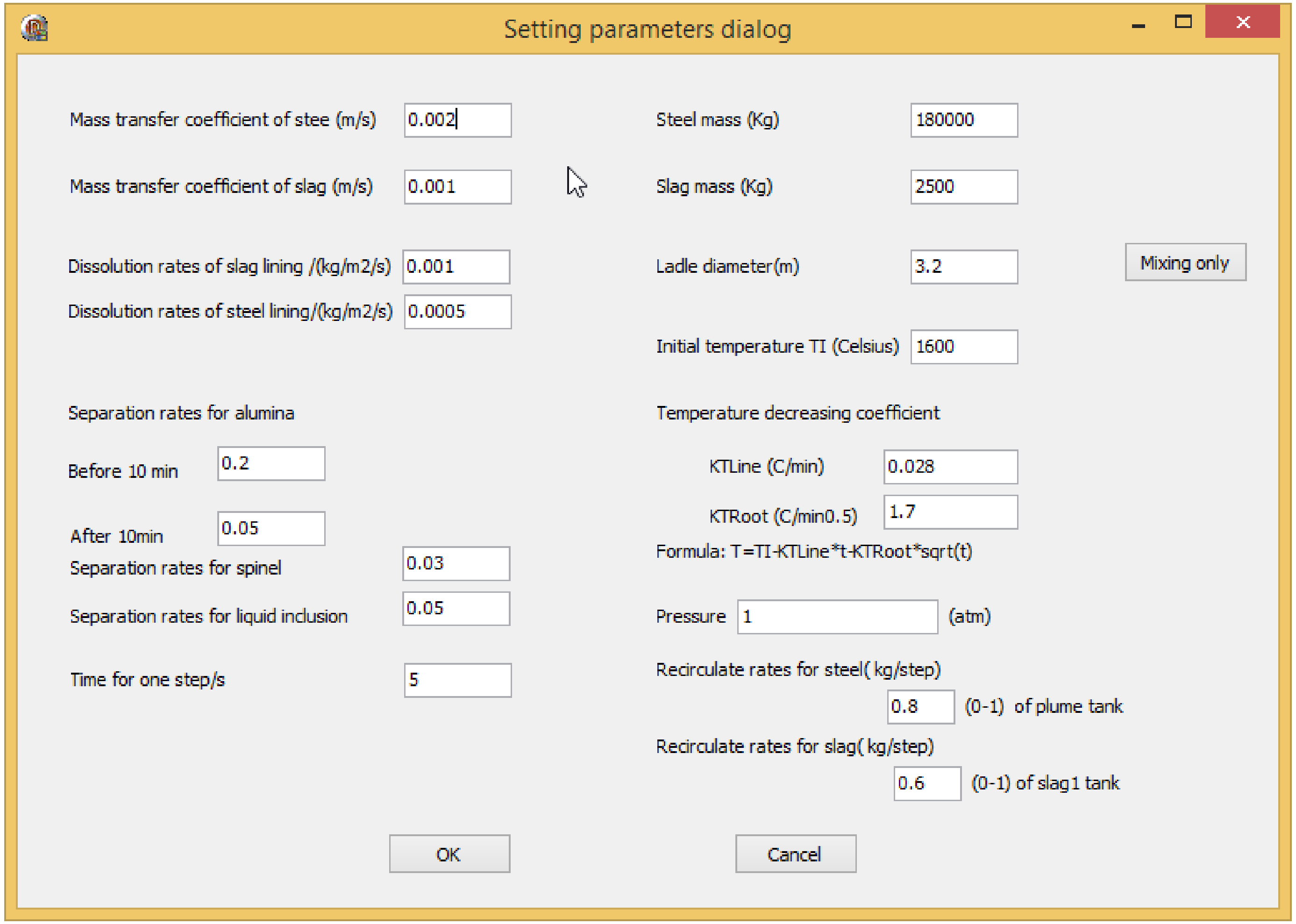
Interface for data input during the process



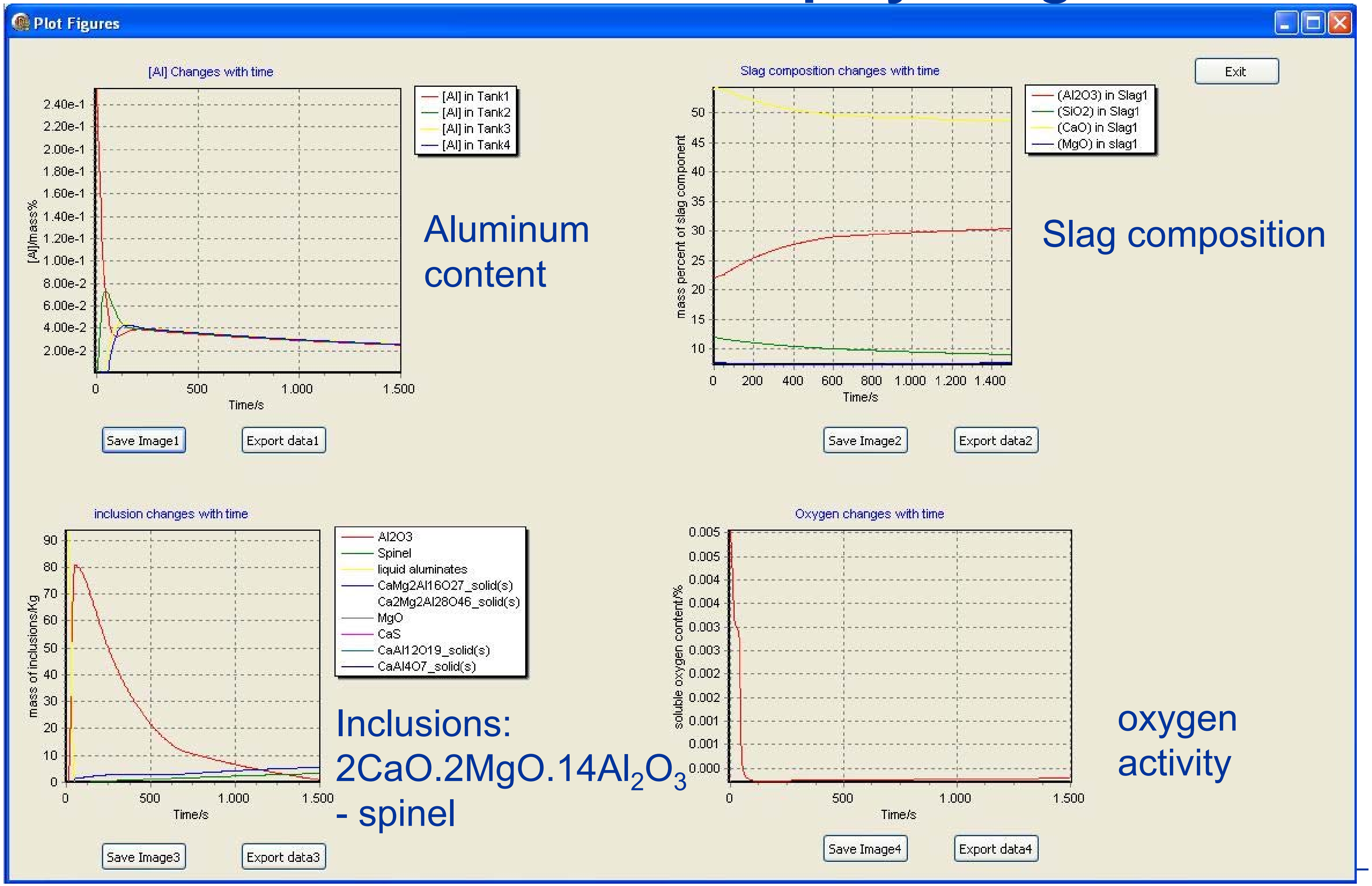
Model parameters
(only for advanced users)

- Mass transfer coefficient (m/s)
  - Steel phase
  - Slag phase
- Dissolution rate/wear of refractory (kg/m^2 s)
  - Steel lining
  - Slag lining
- Separation rates of inclusions
  - Alumina and solid aluminate
  - Spinel
  - Liquid inclusions
- Temperature decrease coefficient/function
- Recirculation rates for steel, stirring function (kg/s)

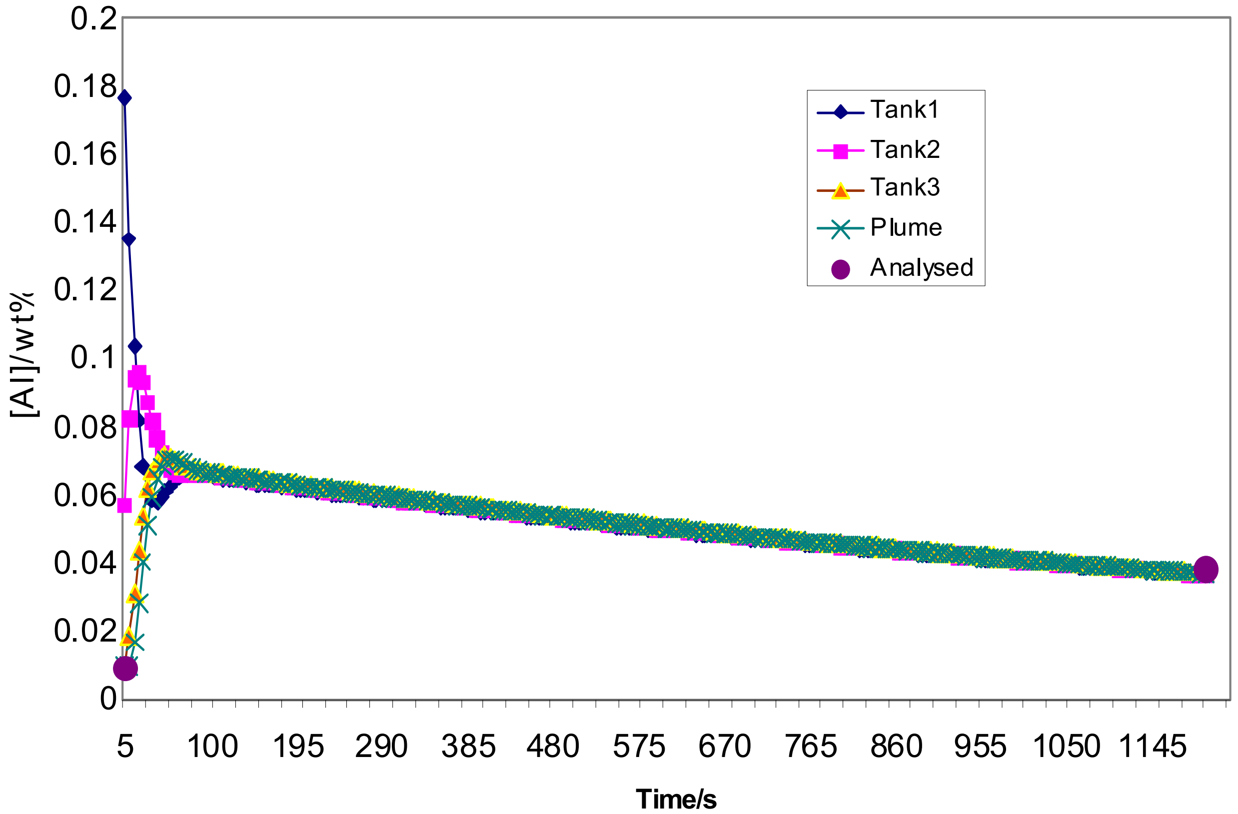
Model parameters dialog window



Process assistance – displayed figures

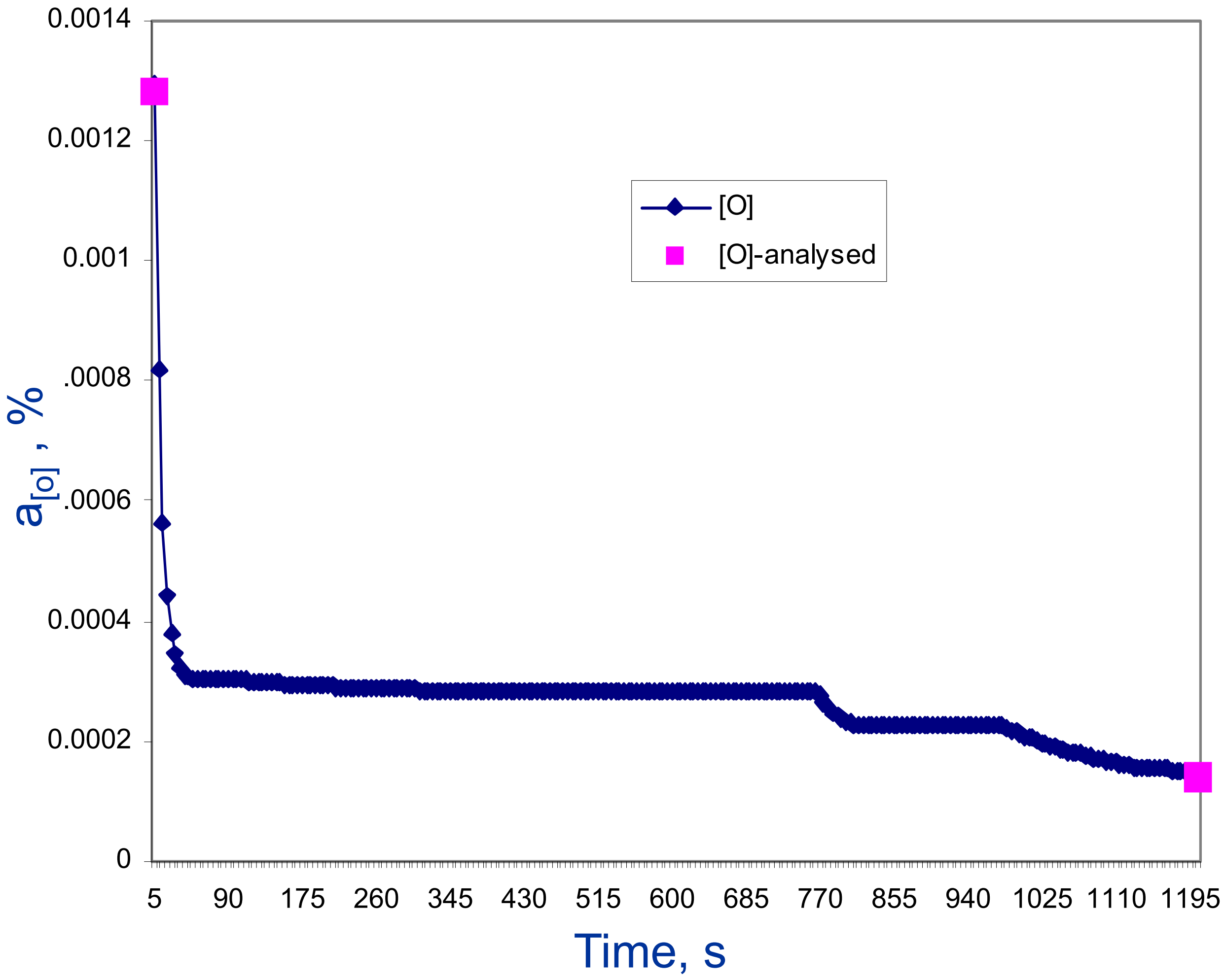


Model Validation



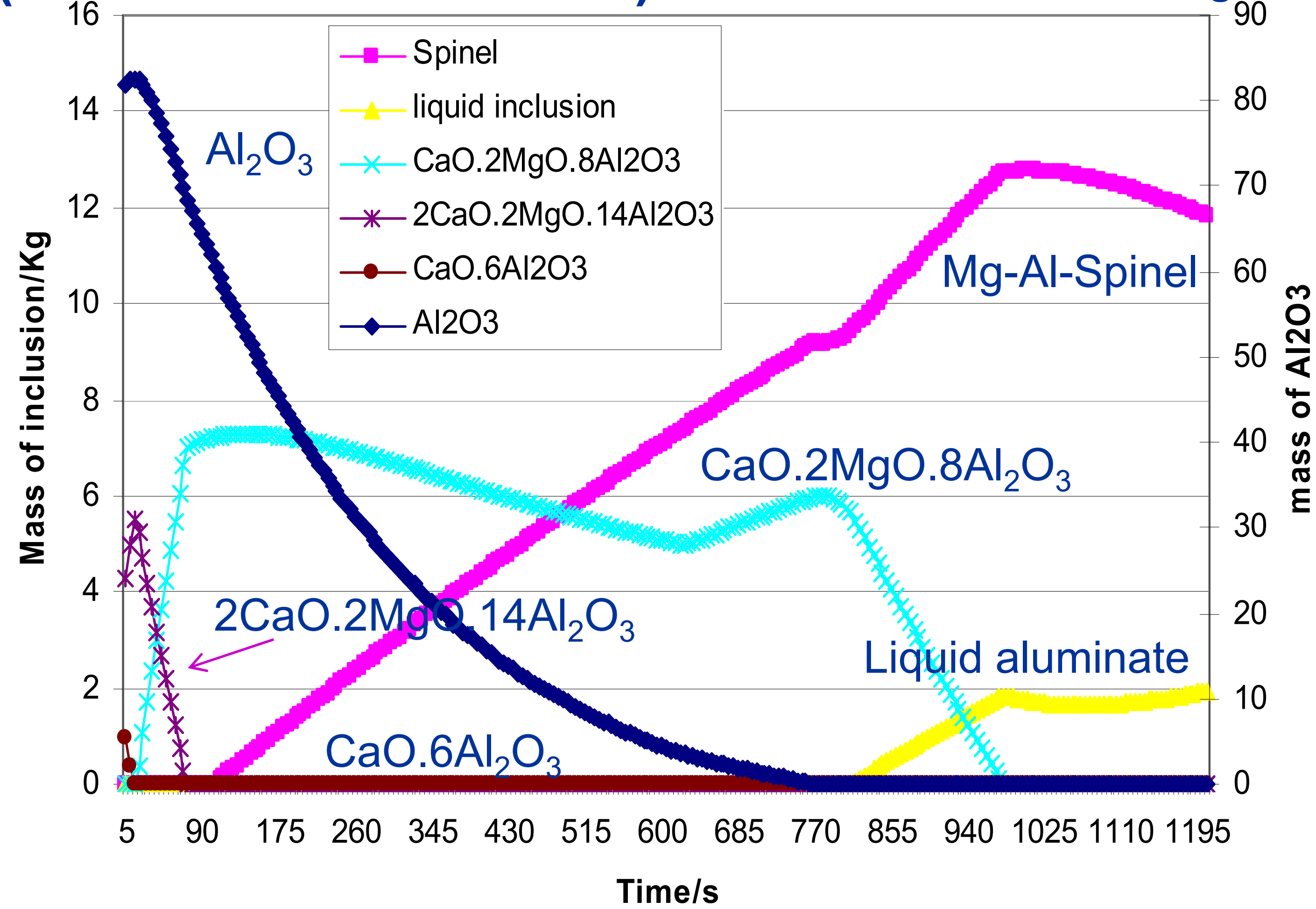
Comparison between calculated [Al] and industrial analysed [Al] during ladle treatment

→ Ladle mixing and slag-metal reaction are dominant factors for [Al] evolution.



Comparison between calculated oxygen activity $a_{[o]}$ and industrial $a_{[o]}$ measurement during ladle treatment. The first drop is due to Al-deoxidation. The other drops could be connected with the seperation and modification of inclusions.

Evolution of inclusions during ladle treatment (before CaSi treatment) calculated; 210t ladle with MgO-C-lining



Major inclusions are alumina, spinel, $CaO.2MgO.8Al_2O_3$. Final inclusions are spinel and some liquid aluminate.

Model Validation

Comparison: inclusions analyzed in ladle samples and calculated inclusions

Process step	Analyzed Inclusions	Calculated Inclusions
Arrival at ladle treatment station	A C D	A C
Before CaSi treatment	B A C	B A C
Departure ladle	C E	E C

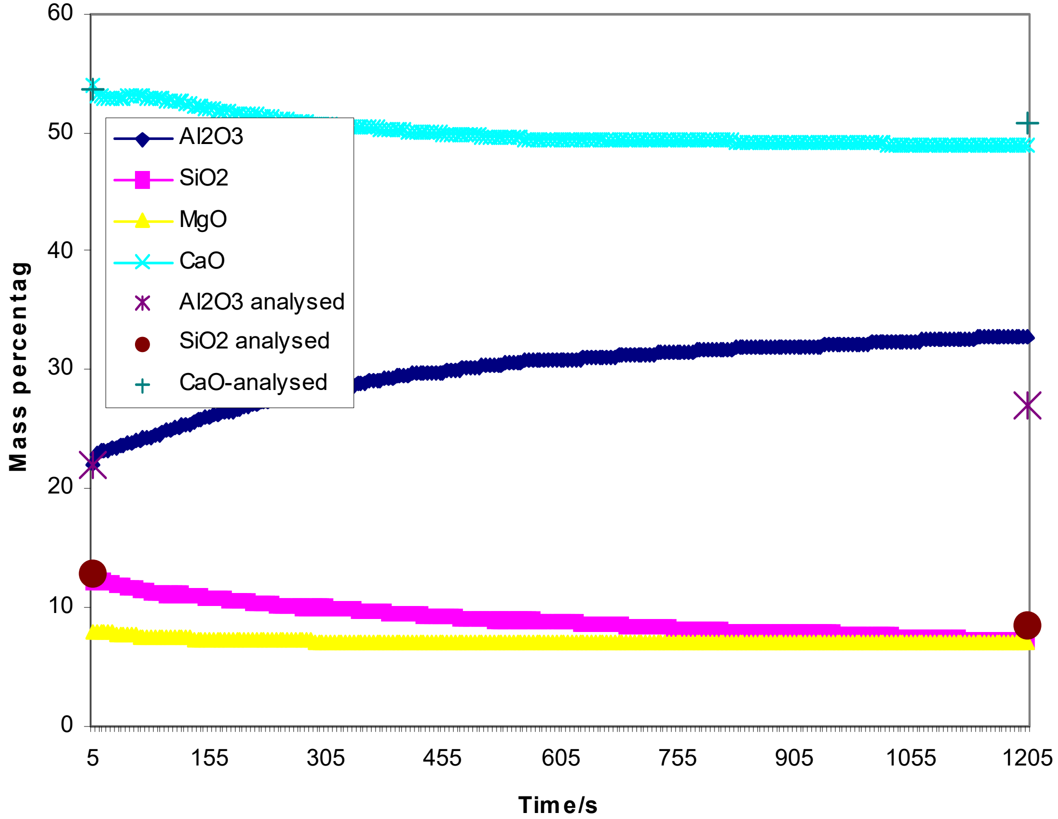
A: Alumina
B: Spinel
C: Calcium aluminate
D: Manganese silicate
E: Calcium sulphide

Inclusions are listed by the amount in decreasing order.

The calculated inclusions before and after CaSi treatment are consistent with inclusion found in industrial sample.

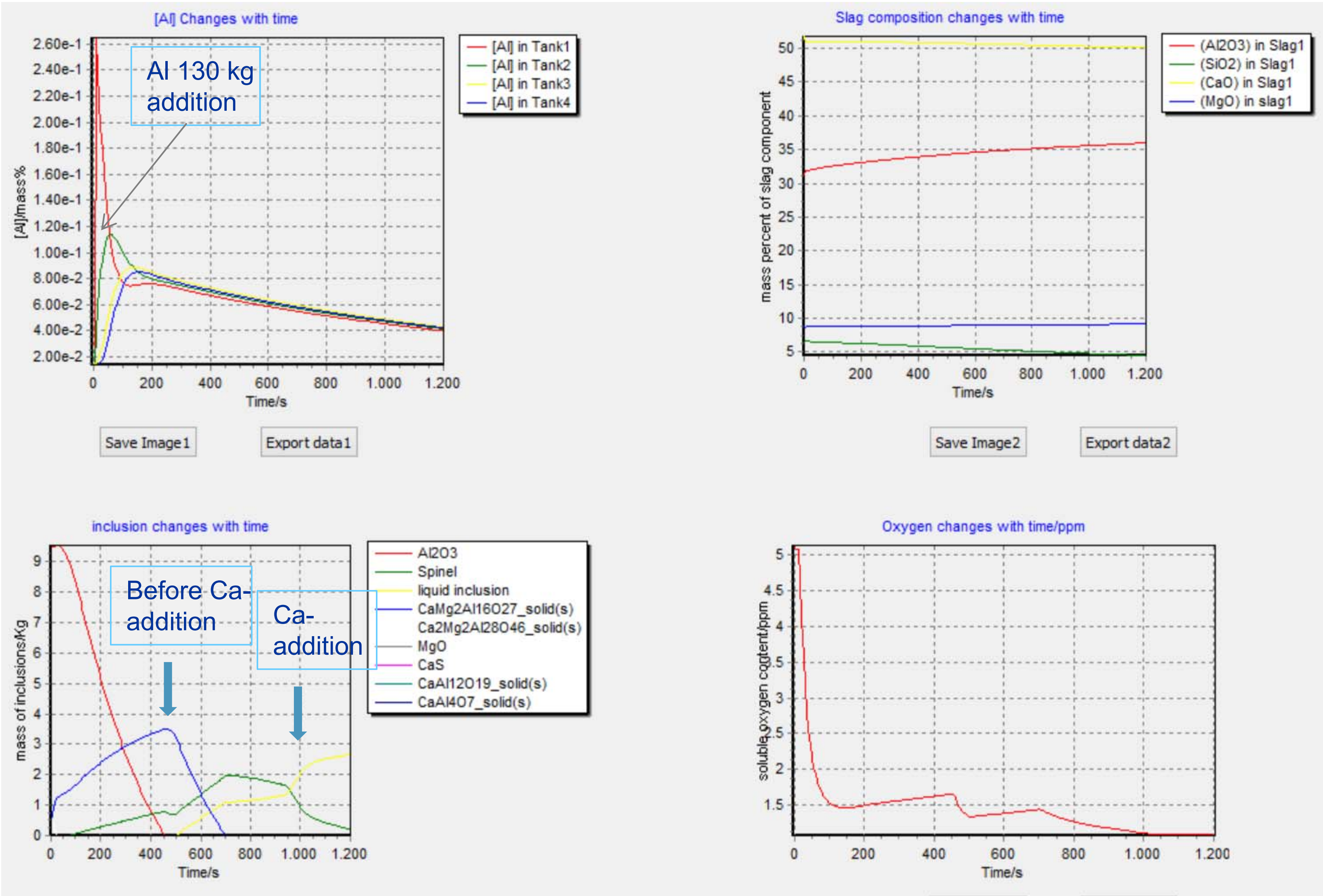
Model Validation

Change of slag composition



Comparison between calculated chemical composition of slag and industrial analyzed compositions during ladle treatment

Standard kinetic conditions, MgO in slag= 8 %, S=60 ppm and **sufficient Ca-addition!**



Model Validation

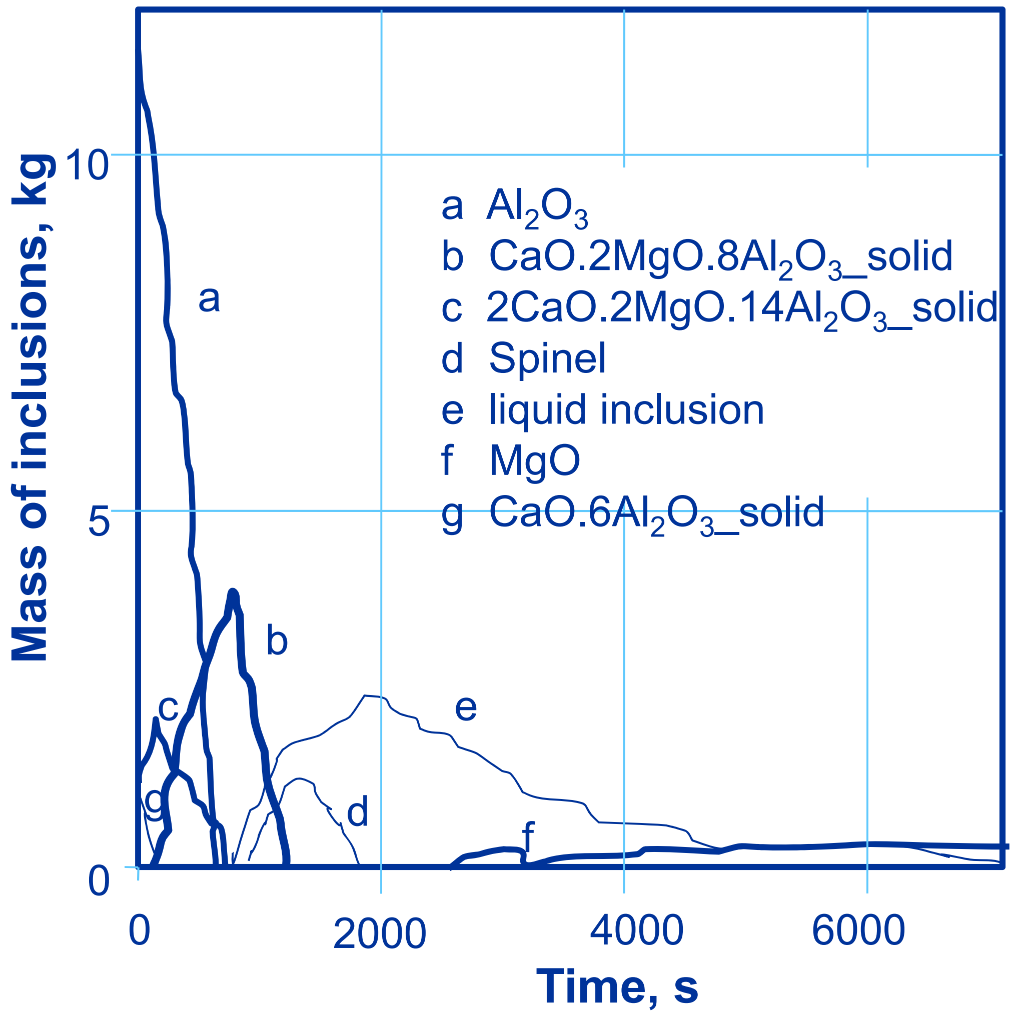
Validation in 30 t ladle, treatment of low alloyed steel

Model Validation

Industrial data for model validation, 30 t melts

Parameter	Mass, composition, additions
Steel and slag mass	Steel: 30000kg, Slag: 250kg
Chemical composition of steel during treatment (used in calculation)	C: 0.24%; Mn: 0.29%; Cr: 1.67%; Mo: 0.39%; V: 0.086%; Si: 0.09%
Chemical composition of slag, after deoxidation and before treatment (starting values)	CaO: 55%; SiO_2: 7%; Al_2O_3: 30%; MgO: 7%; FeO+MnO_2<1%
Deoxidation regime	1) Al after EAF-tapping 2) Al during treatment
Lining	MgO-C

Calculated evolution of inclusions during ladle treatment of 30t heat resistant steel.



Inclusions analyzed during the ladle treatment.

Type No	Inclusion type	Main component	Minor component	Begin ladle furnace	End ladle furnace	Before vacuum degasing
1	pure alumina	Al_2O_3		X		
2	alumina with tracer	Al_2O_3	MnO, SiO_2		o	
3	calcium aluminate	Al_2O_3, CaO		o	X	X
4	spinel	Al_2O_3, MgO	MnO		X	X
5	sulphides	CaS, MnS				o

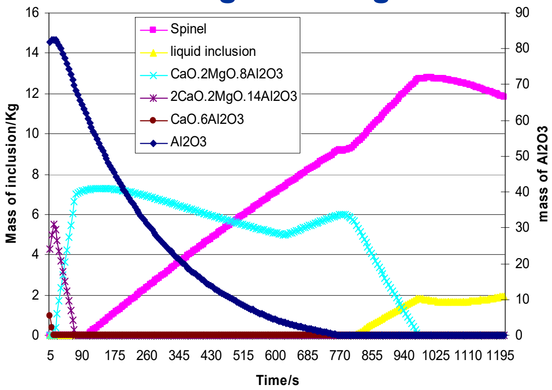
Calculated inclusions at the end of treatment: MgO and liquid Ca-aluminates

X: high quantity,   o: low quantity

Effect of Lining Material (parameter study)

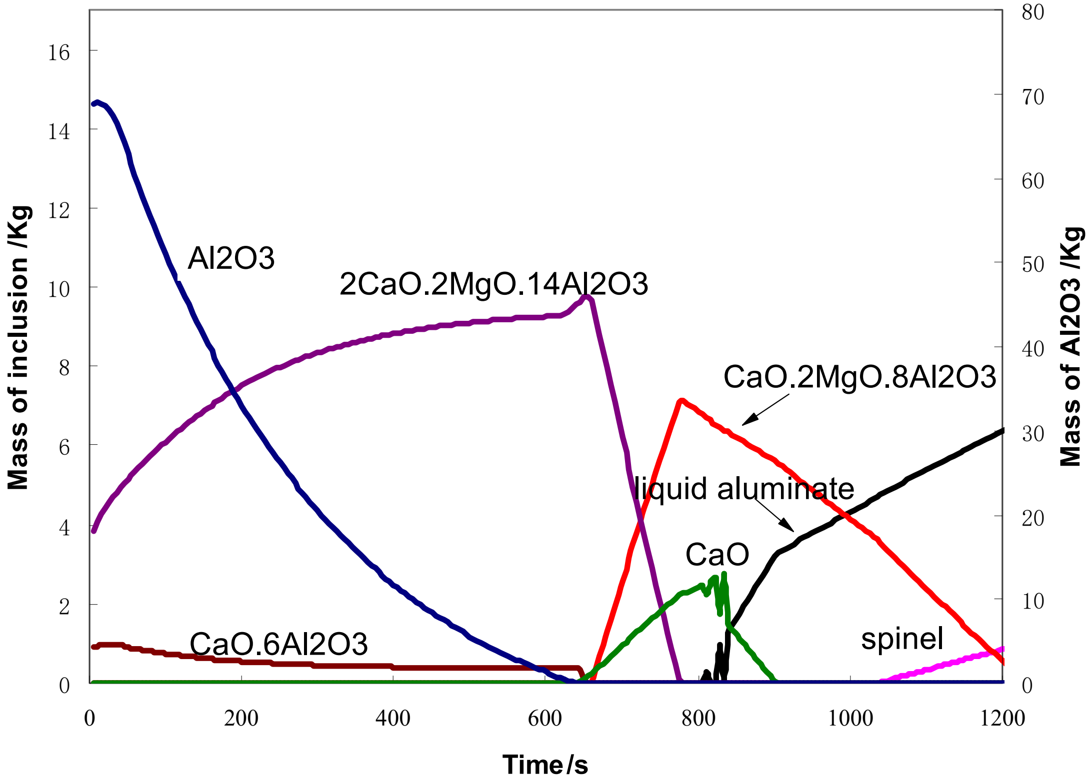
(210t ladle, same conditions, FeO+MnO in the slag negligable)

Inclusion evolution in ladle with **MgO-C lining**



Major inclusions are alumina, spinel, CaO.2MgO.8Al2O3. Final inclusion are spinel and some liquid aluminate

Inclusion evolution in ladle with **dolomite lining**



→ **final inclusions:** liquid aluminates and minor aluminates and Mg-Al spinels; dolomite lining supports the transformation of solid aluminates, spinel into liquid aluminates (by dissolution of Ca into steel and slag)

Conclusion

- A comprehensive model for calculating inclusion composition in gas-stirred ladle, **Clean Steel Control (CSC)** Model, was established by taking into account kinetic parameter estimated in the industrial processes, thermodynamic relationships and several factors.

  Mixing, slag-steel reaction, inclusion separation, lining wear and dissolution were taken into consideration
- The present model can predict inclusion composition consistent with estimated in the industrial practice
- The present model provides good predictions for compositions of slag and steel

Publication

FULL PAPER

steel research international

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Inclusion Development in Steel During Ladle Metallurgical Treatment - A Process Simulation Model – Part: Industrial Validation

Piotr R. Scheller* and Qifeng Shu

Steel cleanliness strongly affects the properties of the products. There is an ever increasing requirement of strict control of inclusion composition and amount during ladle treatment. A comprehensive model for inclusion development in gas stirred ladles developed by the authors is validated in the industrial ladle treatment processes. It can be used for the process simulation and optimization. The important factors, like stirring intensity, reaction between steel and slag as well as refractory material, and the conditions needed for separation and floatation of non-metallic inclusions are taken into account. FactSage and SimuSage packages are employed as the thermodynamics database and simulation tools, respectively. The evolution of steel and slag composition along with the amount and composition of inclusions during the ladle treatment are calculated and compared with results from the industrial process. The comparison between model predictions and actual plant data shows good agreement as well for 210 t heats as for 30 t heats and different steel grades. The present model is a useful tool for simulation and optimization of ladle metallurgical treatments in industry.

1. Introduction

The improvement of steel quality is one of most important tasks for researchers in the field of process metallurgy.

separate out into slag phase. The composition of inclusions gradually changes due to reaction with elements like Ca and Mg added to steel. Reactions which take place at the interface between top slag and steel can

Piotr R. Scheller and Qifeng Shu, steel research international, vol 85 (2014), No. 8, pp. 1310 – 1316

Thank you

Clean Steel Control (CSC)

Model

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