



Application of FactSage and SimuSage calculations in research and education within Process Metallurgy at Luleå University of Technology

**Bo Björkman, Andreas Lennartsson, Fredrik
Engström, Caisa Samuelsson**

**Minerals and Metals Research Laboratory
Luleå University of Technology**

Outline

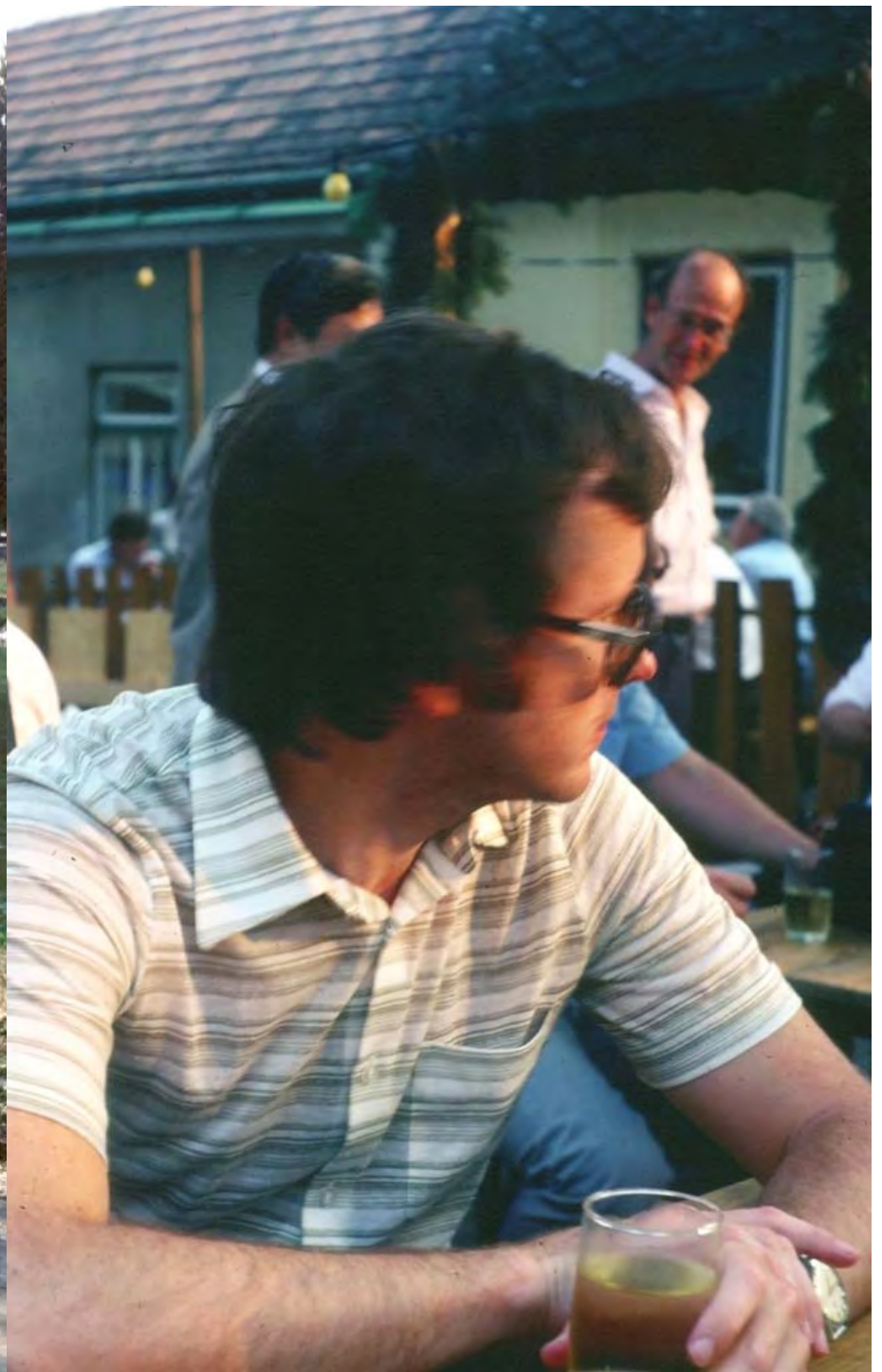
- **Earlier activities on process modelling**
- **Research within Process Metallurgy at LTU**
- **Process modelling of a copper converter**
- **Leaching from steelmaking slag**
- **Application of slag in cement applications**
- **Conclusions**





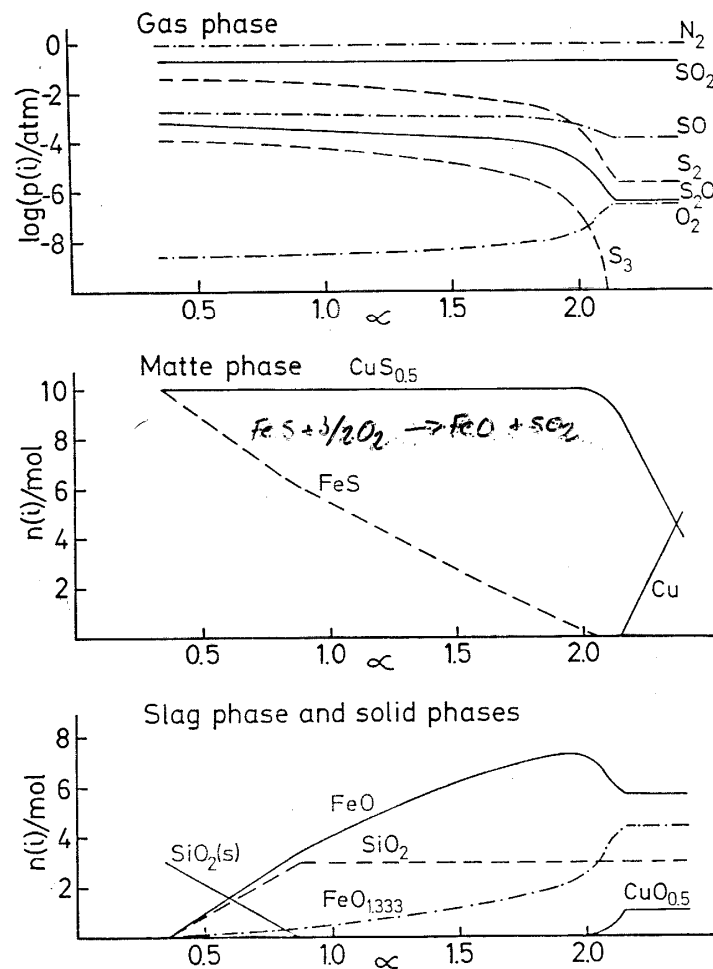
- Supervisor during PhD study
- Teacher in thermodynamics
- Introduced me to SOLGASMIX
- Good friend

Thank You and the very
best for the future!

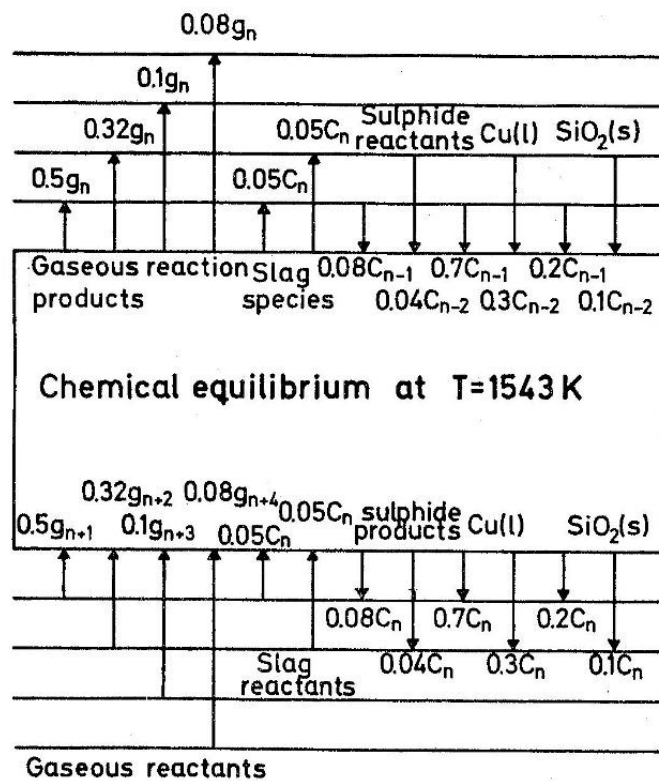


Use of Solgasmix in the 80's

Calculations on smelting and converting of copper



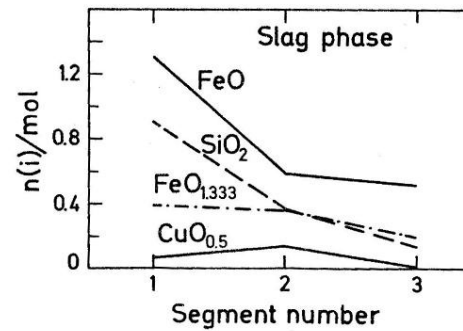
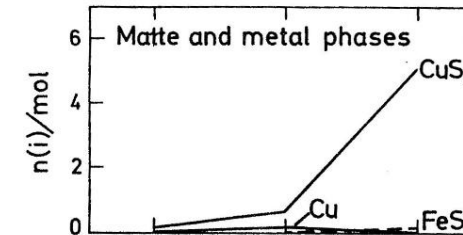
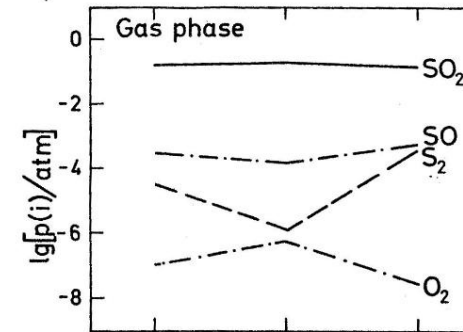
Björkman B, Eriksson G, Quantitative Equilibrium Calculations on Conventional Copper Smelting and Converting, Can. Metall. Q., 21, 1982, 329-37.



Segment number
n - 4
n - 3
n - 2
n - 1

n

n + 1
n + 2
n + 3
n + 4



Björkman, B, Quantitative equilibrium calculations with relevance to copper making, Thesis, Umeå University, 1984, Supervisors Gunnar Eriksson and Erik Rosén



Process simulations during 80's at Boliden and at LTU.

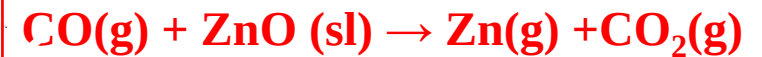
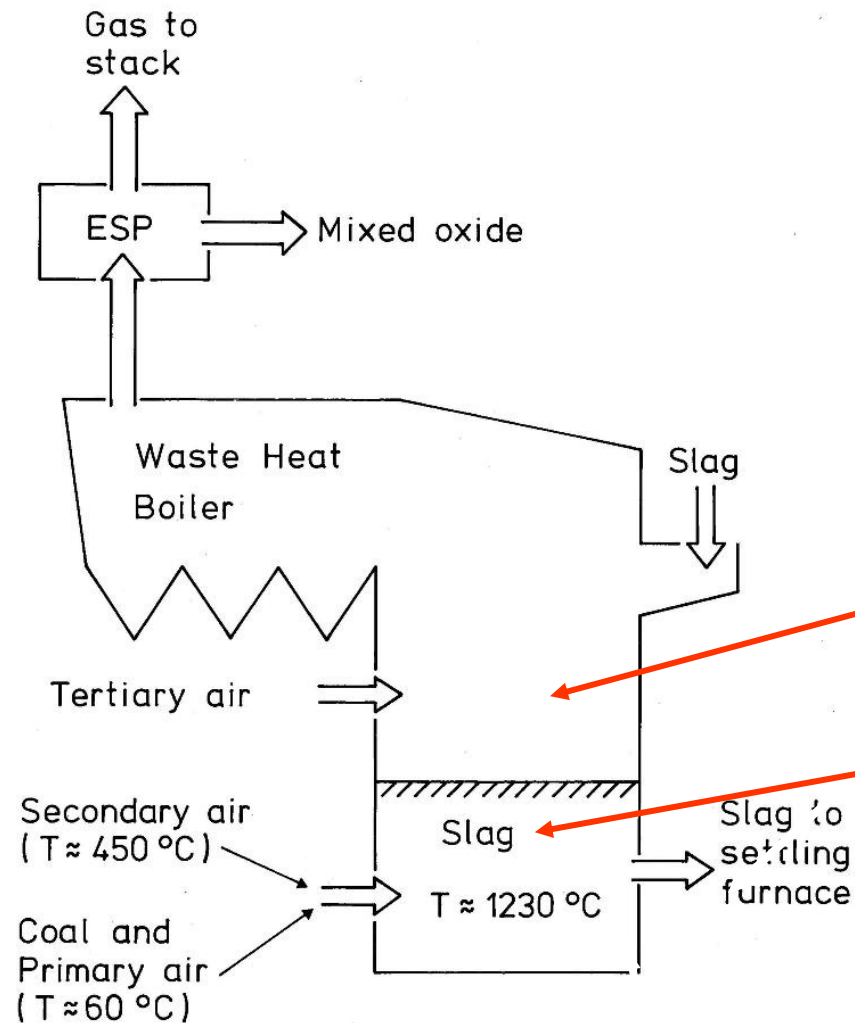
A simple data file for the system **Cu-Fe-O-S-Zn-Pb-Ni-As-Sb-Bi-Sn-Ag-CaO-SiO₂-Al₂O₃-(Cl-C)**, including solution models for slag, matte and liquid metal phases.

Applied to:

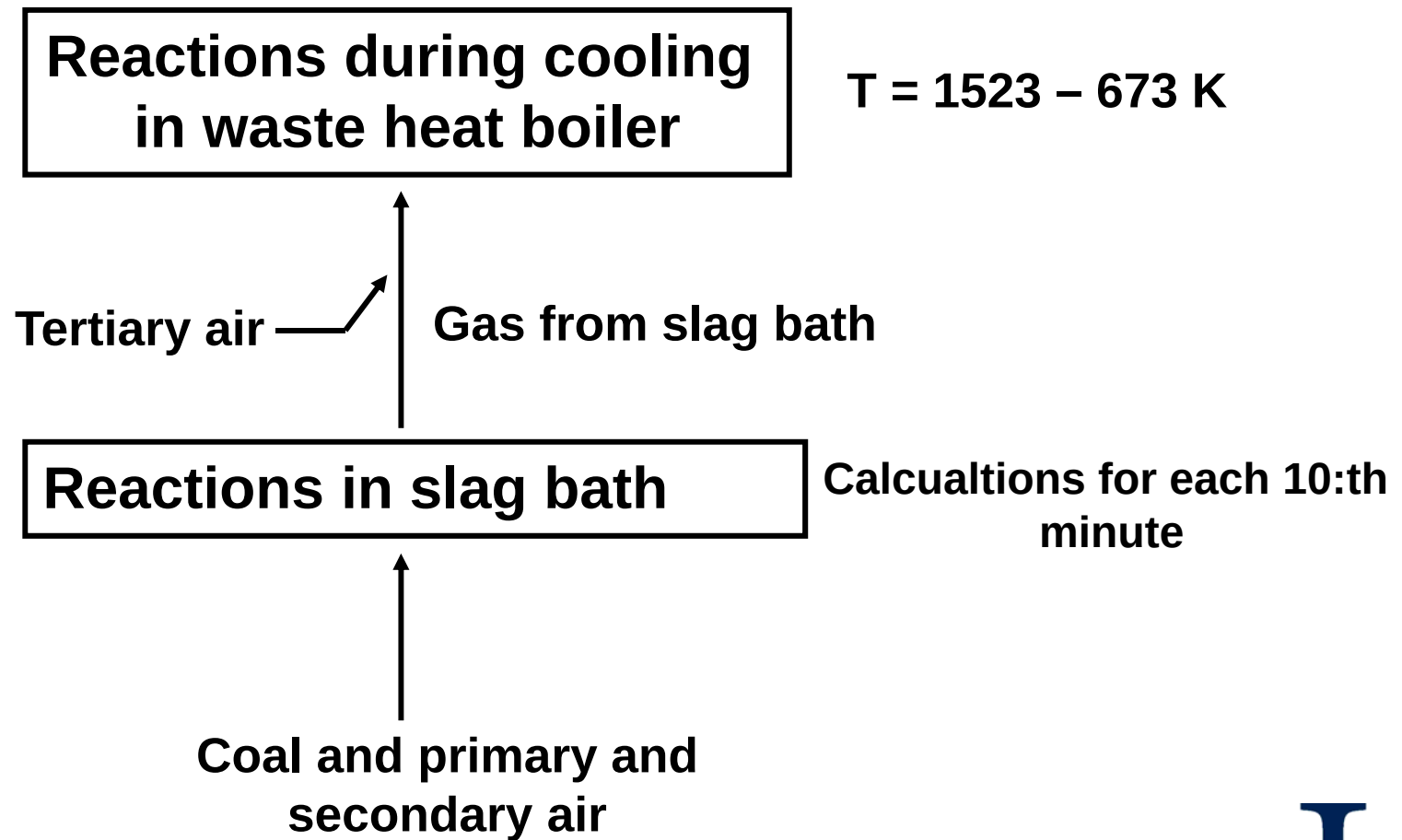
- Roasting of copper concentrates
- Calculations on chlorinating roasting
- Simulation of zinc fuming plant
- Smelting of copper containing scrap in a Kaldor furnace (TBRC)
- Smelting and converting of anode slime in a Kaldor furnace (TBRC)
- Gas composition during copper converting
- Impurity distribution during smelting and converting

Example:

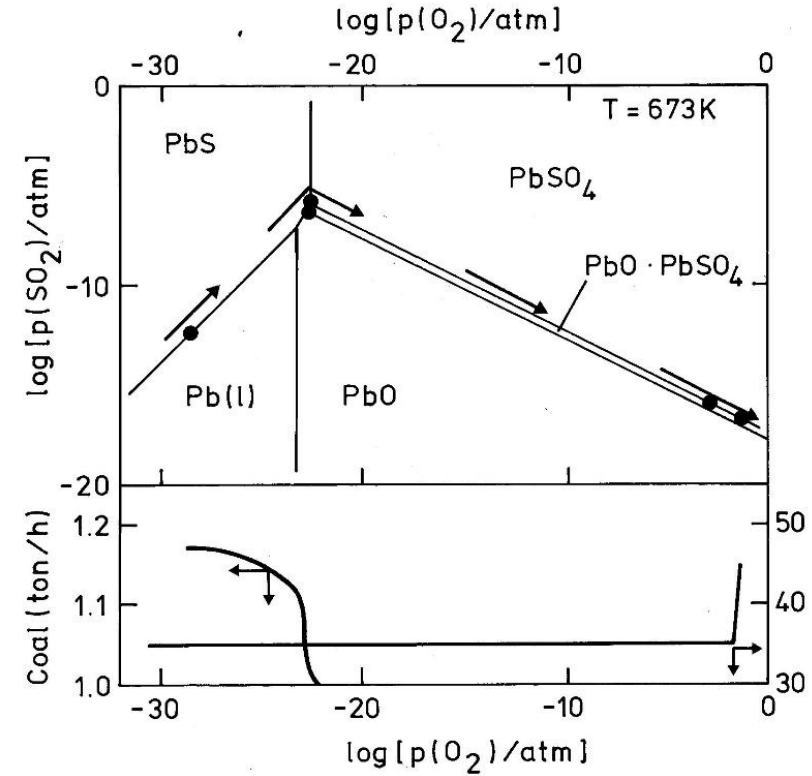
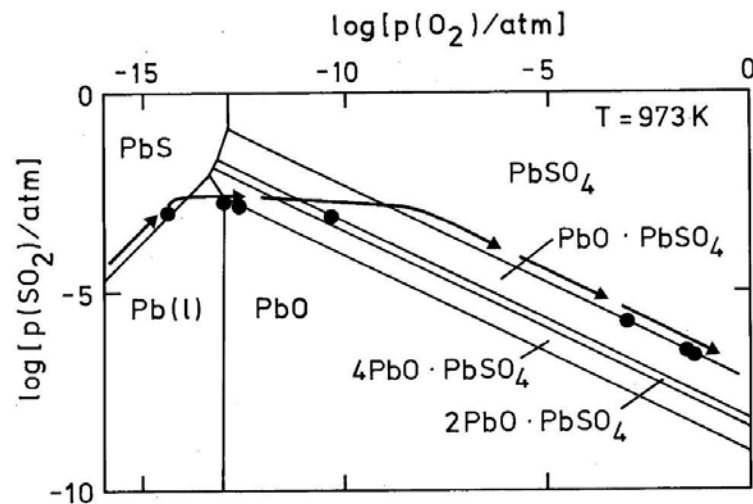
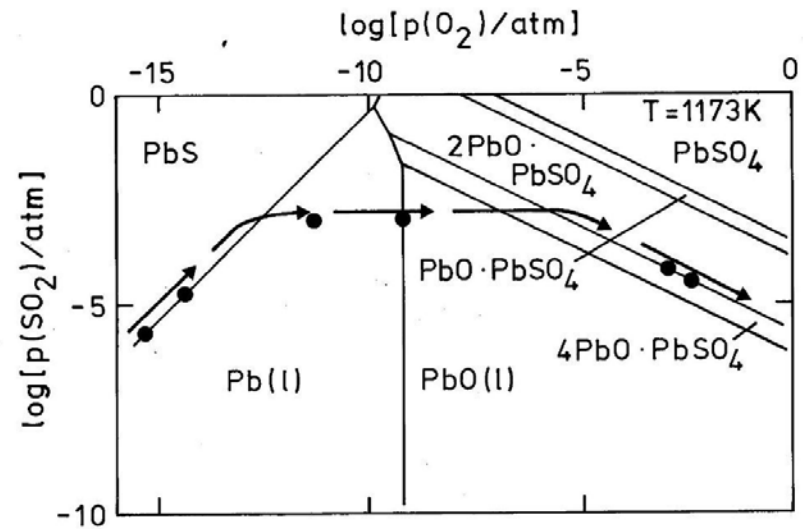
Dust formation in the zinc fuming plant at
Boliden AB, Rönnskärsverken



Calculation procedure



Results on formation of condensed lead phases during cooling of the process gas





Research within Process Metallurgy at LTU

MiMeR, Minerals and Metals Research Laboratory:

Two research subjects: **Process Metallurgy** Mineral Processing

Six full professors:

Process Metallurgy Mineral Processing Surface chemistry

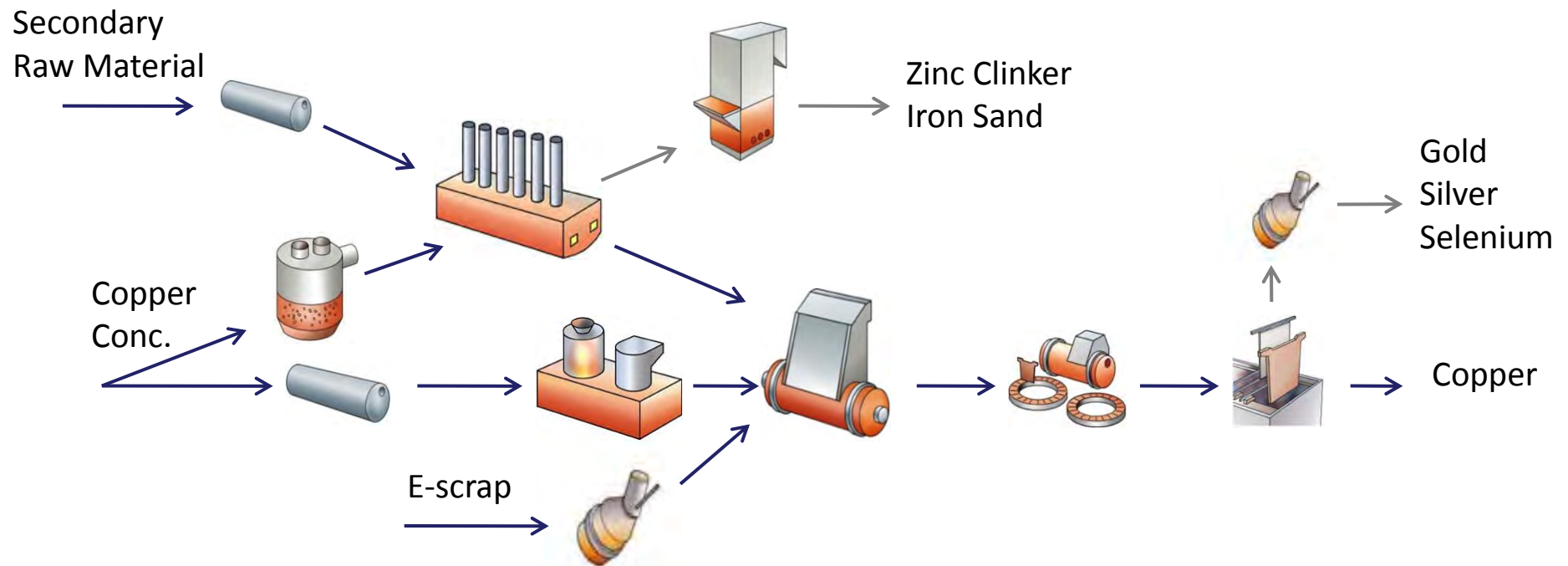
Hydrometallurgy **Sustainable Production of Iron Ore** GeoMetallurgy

Application Areas related to Process Metallurgy:

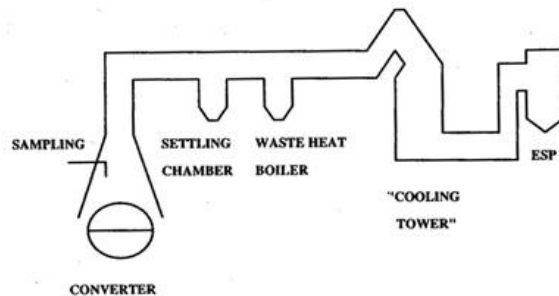
Base metals production Iron making Bio-hydrometallurgy
Recycling and Residue utilisation

Simulations connected to a PS-copper converter

Copper flow at Bolidens Rönnskär smelter



Simulation of dust formation in the dust cleaning system of a PS-Converter



**AVERAGE COMPOSITION OF DUST,
FIGURES GIVEN IN WEIGHT %**

	CONVERTER HOOD, FINE FRACTION	SETTLING CHAMBER	WASTE HEAT BOILER	COOLING TOWER	ESP
Cu	1	26	22	22	0.8
Fe	0.4	3	2	3	0.2
SiO₂	-	31	38	15	0.7
Pb	42	4	15	16	42
Zn	11	2	5	6	10
As	4	0.25	1	2	6.5
Bi	1	0.08	0.5	0.5	1.5
S	8	8	10	12	9

Condensation from gas versus amount of leakage air at equilibrium conditions



T/K	No leakage air	5% leakage air	100% leakage air
1423		ZnO	ZnO
1323	ZnS	PbSO ₄ Bi ₂ O ₃	PbSO ₄ Bi ₂ O ₃
1223			Sb ₂ O ₄ PbSO ₄ Bi ₂ (SO ₄) ₃
1123	PbS	Sb ₂ O ₄ PbSO ₄ Bi ₂ (SO ₄) ₃	
1023			
923	PbS Sb ₂ S ₃ Bi ₂ S ₃		
823			
723			
623	As ₂ S ₃ As ₂ O ₃		
523		As ₂ O ₅	As ₂ O ₅

POSSIBILITIES TO OBTAIN A CONTROLLED DUST GENERATION

CONVERTER GAS WITH
NO OR A LIMITED AMOUNT
OF LEAKAGE AIR

↓
**GAS CLEANING
AT T > 900°C** MECHANICAL
DUST AND ZN

↓
COOLING

↓
T < 600°C
**GAS CLEANING
AT LOW TEMP.** CHEMICAL DUST
e.g. PB, AS, SB



Challenges in modelling a P.S. Converter

Characterised by:

Non-ideal behavior

Non-equilibrium process

Minor elements not assessed for the system

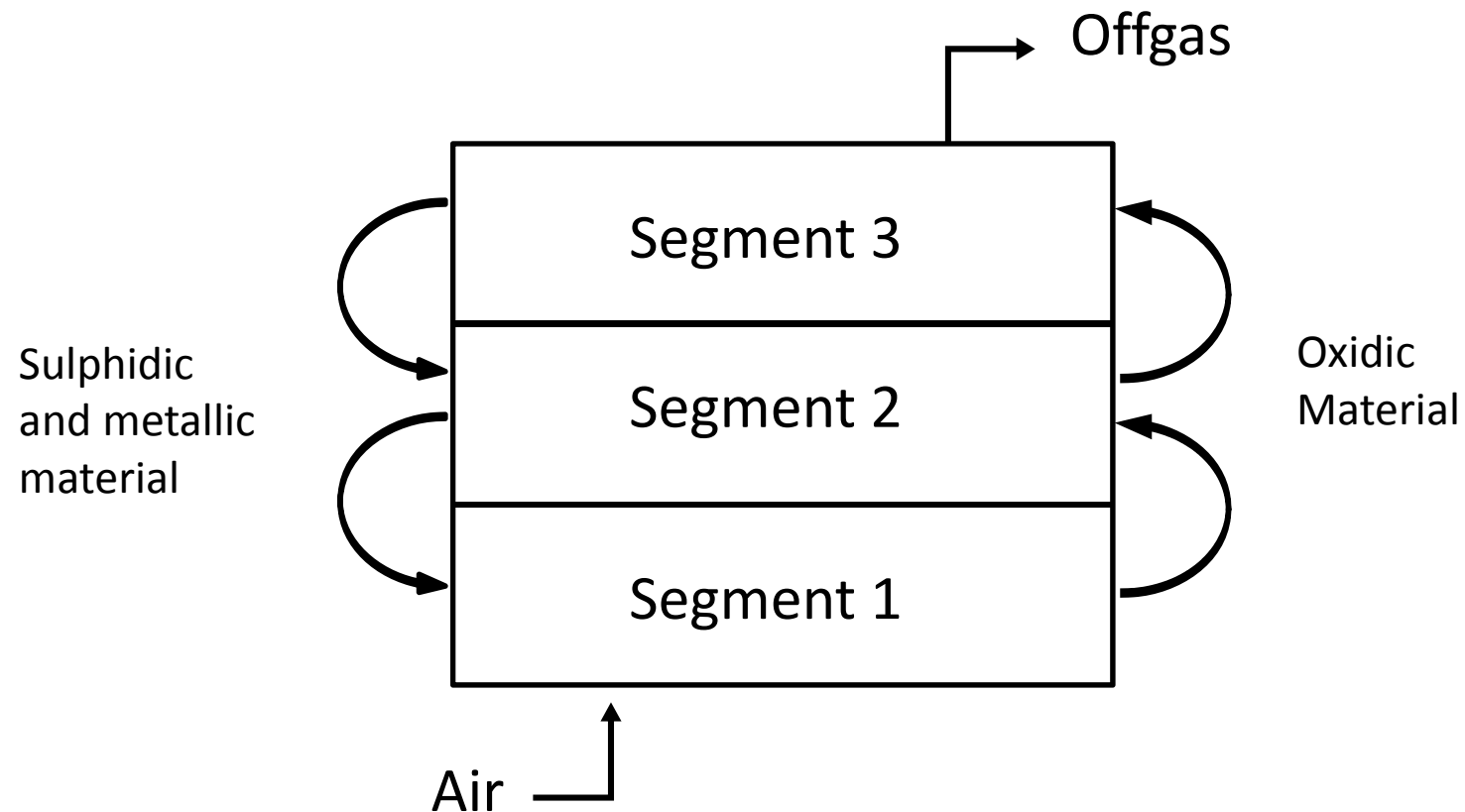
More than obvious phases (e.g. several mattes, immiscible slags, dispersions)

Challenges

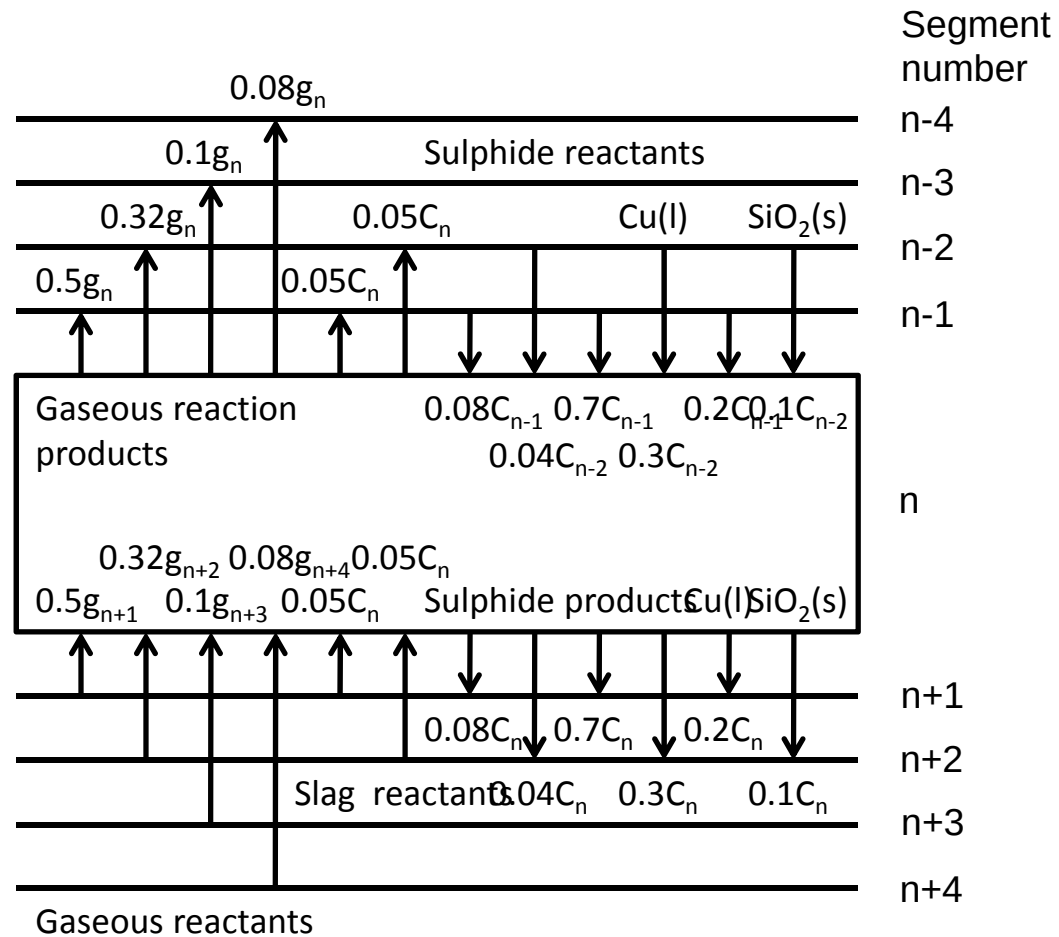
How to include non-equilibrium

Include minor elements to liquid sulphide, slag and liquid metal

Include Non-equilibrium



Include Non-equilibrium



Some comparisons between plant data and calculated values – the slag composition

		Liquid slag					
		Fe	Cu	Pb	Zn	S	SiO ₂
Charge	Plant data	31.2	6.1	6.5	6.6	-	29.9
860	Model prediction	34.4	5.0	4.0	9.5	0.0	30.0
Charge	Plant data	30.4	7.9	7.9	5.2	0.5	30.8
864	Model prediction	29.8	7.4	10.5	5.5	0.0	31.9

The white metal



		White metal				
		Fe	Cu	Pb	Zn	S
Charge	Plant data	0.4	75.9	0.5	0.1	17.8
860	Model prediction	1.1	75.9	1.7	0.6	20.0
Charge	Plant data	0.3	75.9	0.6	0.1	17.7
864	Model prediction	1.0	75.9	1.8	0.7	19.8

Conclusion from modelling of PS-converter

- **The complexity of scrap like WEEE and residue materials calls for new better process models.**
- **By introducing reactor segments into the model, the non-equilibrium conditions can be simulated.**
- **Need for better thermodynamic description for minor and micro elements in the system.**

Leaching from steelmaking slag -

Water granulation

Hypothesis

Fast cooling -> formation of a glass -> enclosing the metals



Ovako EAF slag granulated 031015

Reactivity increases in most cases!

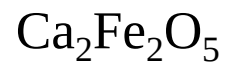
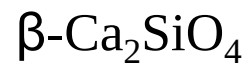
Element	LD slag			EAF slag		
	α		(Rapid)/(Semi) %	α		(Rapid)/(Semi) %
	Semi-rapid cooling	Rapid cooling		Semi-rapid cooling	Rapid cooling	
Ca	1,87E+00	9,86E+00	526%	2,90E-01	2,69E+00	928%
Na	1,87E-03	2,89E-02	1543%	1,09E-03	3,09E-02	2824%
S	4,62E-03	1,06E-01	2305%	2,55E-03	1,52E-02	596%
Si	6,34E-03	2,98E-01	4694%	6,30E-02	7,78E-01	1235%
Al	8,15E-03	7,76E-03	95%	2,30E-03	1,61E-02	701%
Ba	1,75E-04	8,93E-04	510%	2,67E-04	4,05E-04	151%
Cr	3,29E-06	1,74E-04	5284%	3,68E-04	5,50E-03	1494%
Mn	4,23E-05	3,99E-05	94%	6,26E-06	5,23E-05	835%
Mo	2,79E-05	3,11E-04	1117%	4,82E-05	3,84E-04	797%
V	2,98E-04	3,67E-02	12317%	1,24E-03	1,79E-03	144%

Two examples of EAF slag

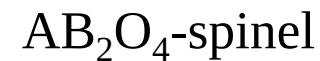
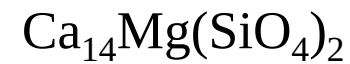
	Type 1 Low all.	Type 2 High all.
CaO	28.8	41.0
SiO ₂	11.8	28.4
MgO	8.5	4.7
FeO	25.5	2.2
MnO	6.1	3.2
Al ₂ O ₃	4.9	10.1
Cr ₂ O ₃	3.5	5.7
Fe _{met}	4.8	0
B ₂	2.4	1.4

Common minerals in EAF slags

Type 1



Type 2

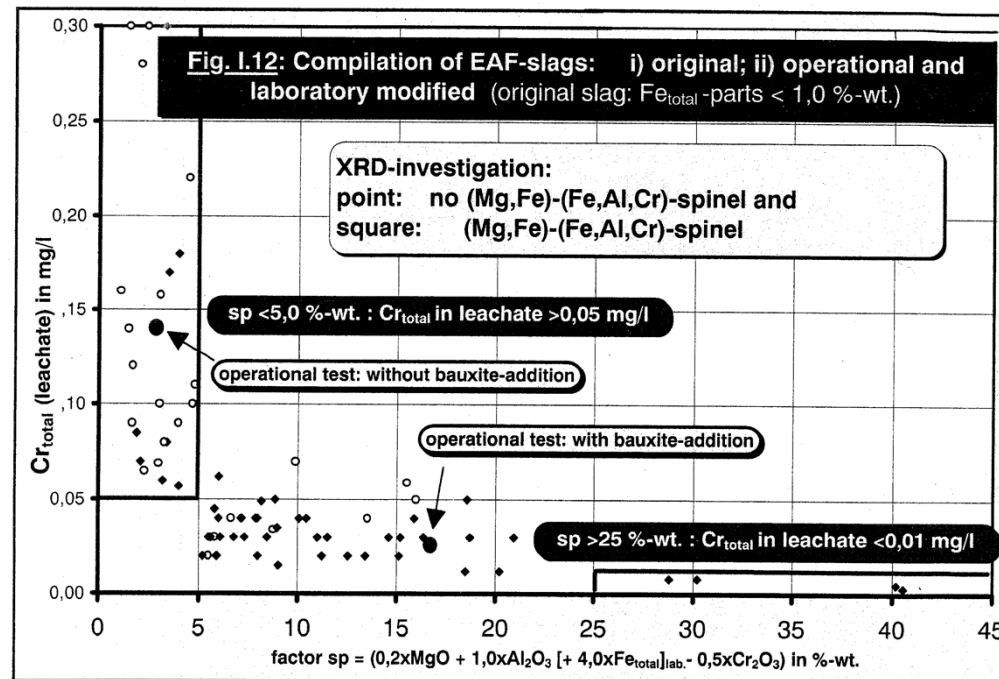


Leaching of chromium might be a problem for the utilization of the slag!

The spinell factor to describe leaching of Cr from steelmaking slag (FEhS ,Year 2000)

$$sp = 0.2MgO + 1.0Al_2O_3 + nFeOx - 0.5Cr_2O_3$$

n' is a number between 1 and 4, depending on the oxidation state of the slag.



Chromium in EAF slag

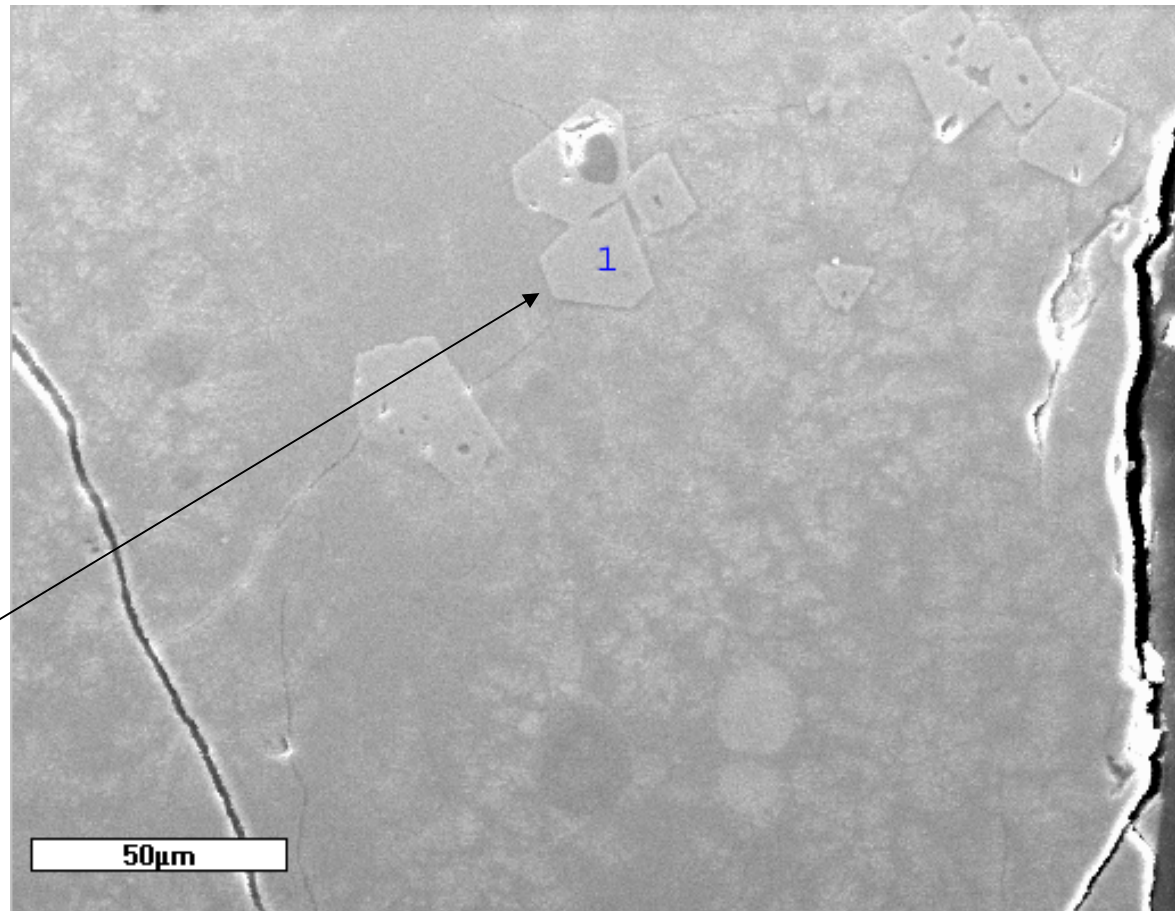


EAF slag type 1

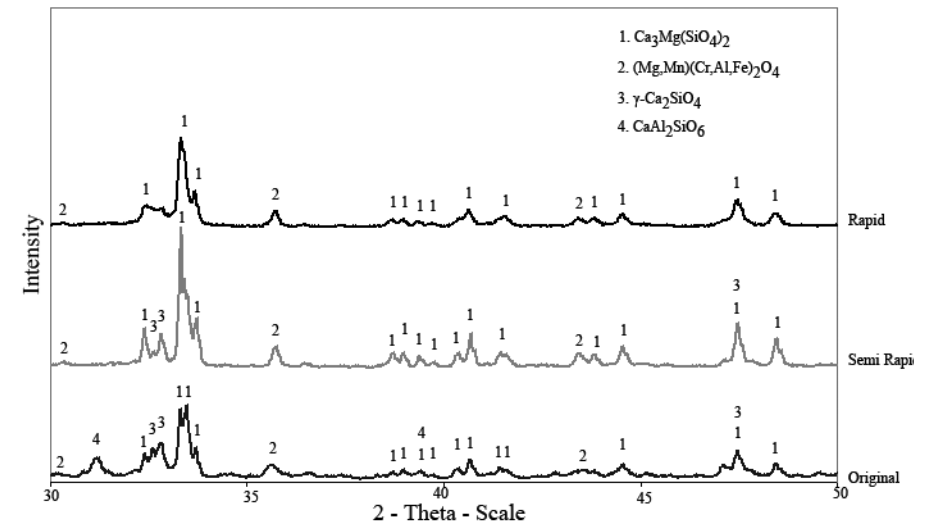
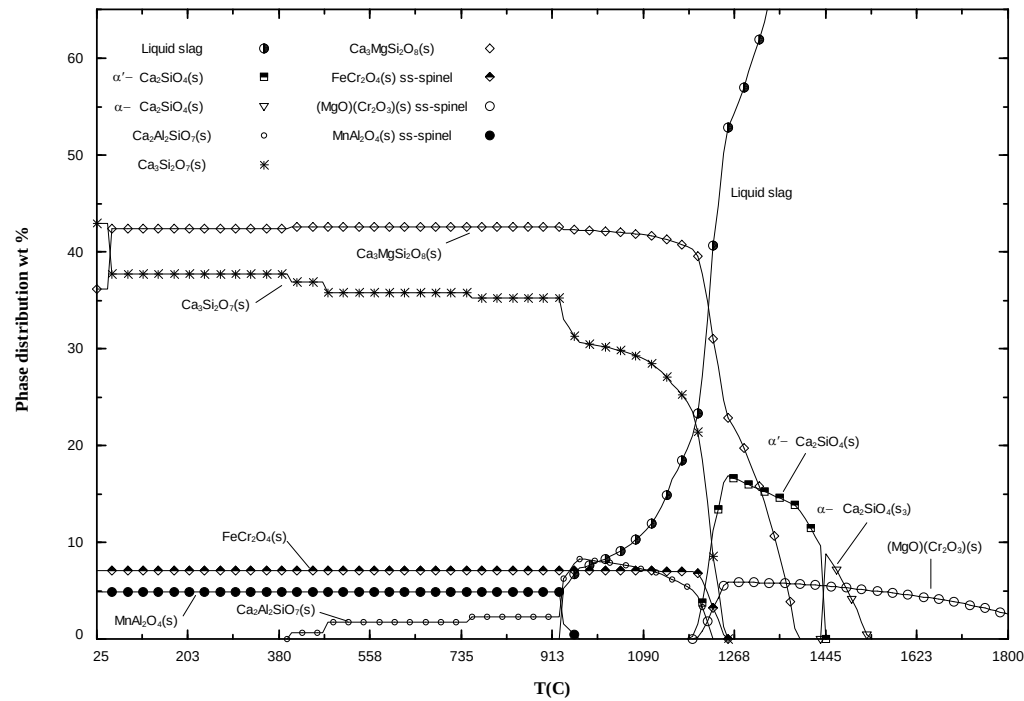
Sp-factor not working

EAF slag type 2

Sp-factor working



EAF slag, type 2



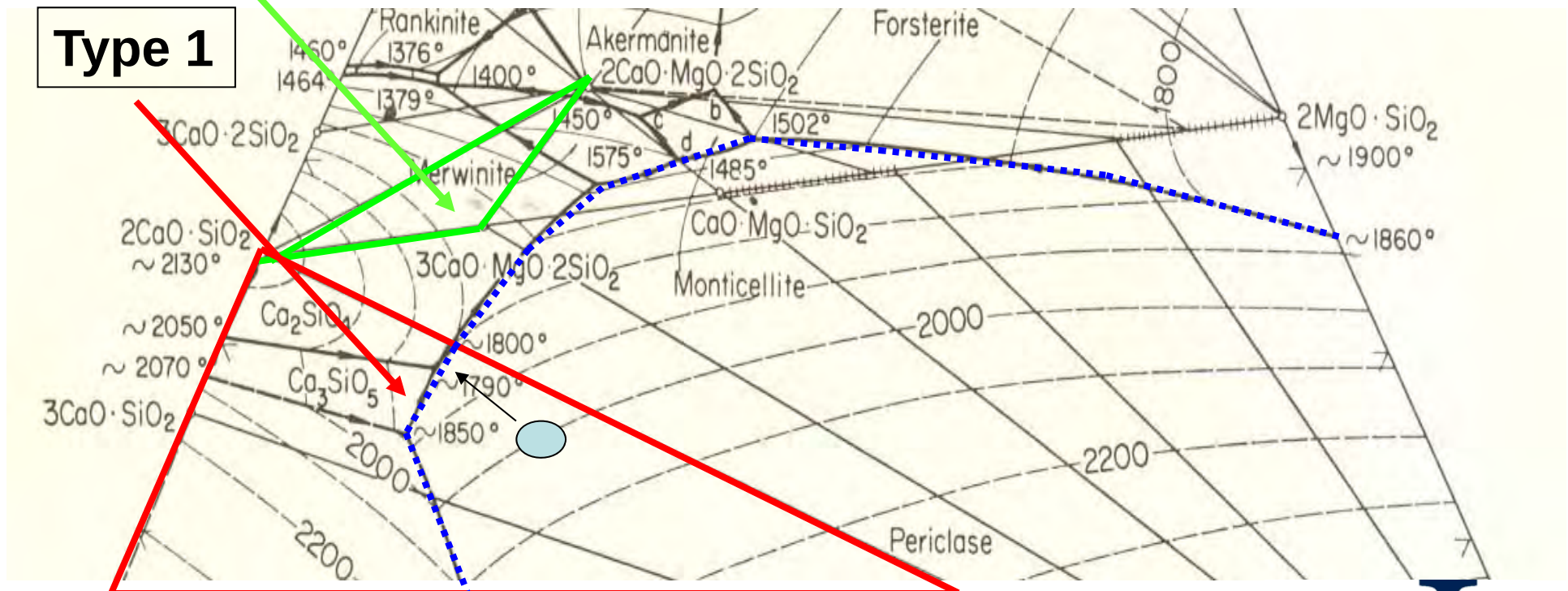
Chromium in EAF slag

Type 2

Why is not sp-factor working for EAF 1 (Carbon steel)?

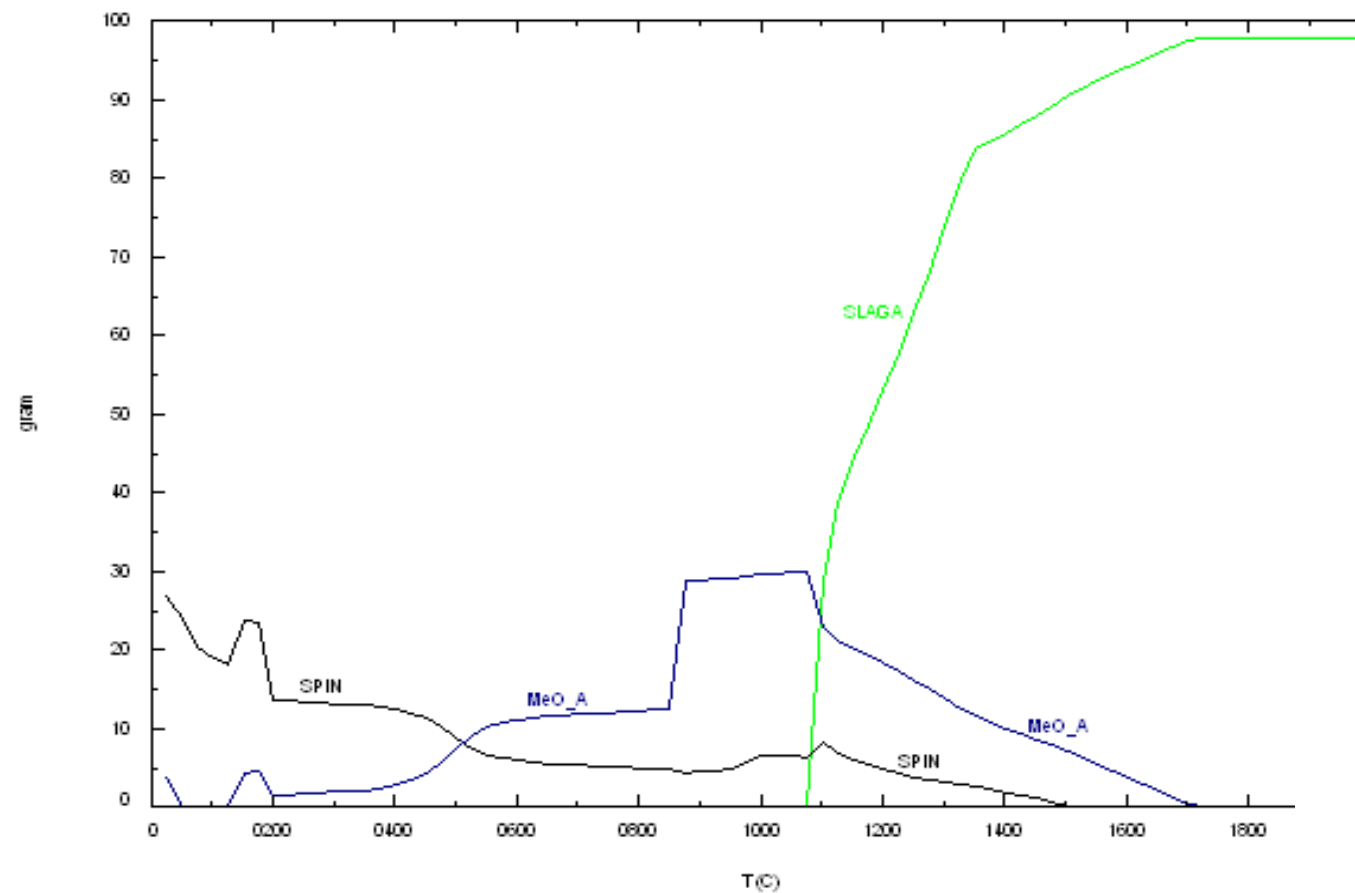
Most important factor to consider – primary crystallisation

Type 1



EAF slag, type 1

Ovako EAF "Liquid slag, MeO_A, Spin"

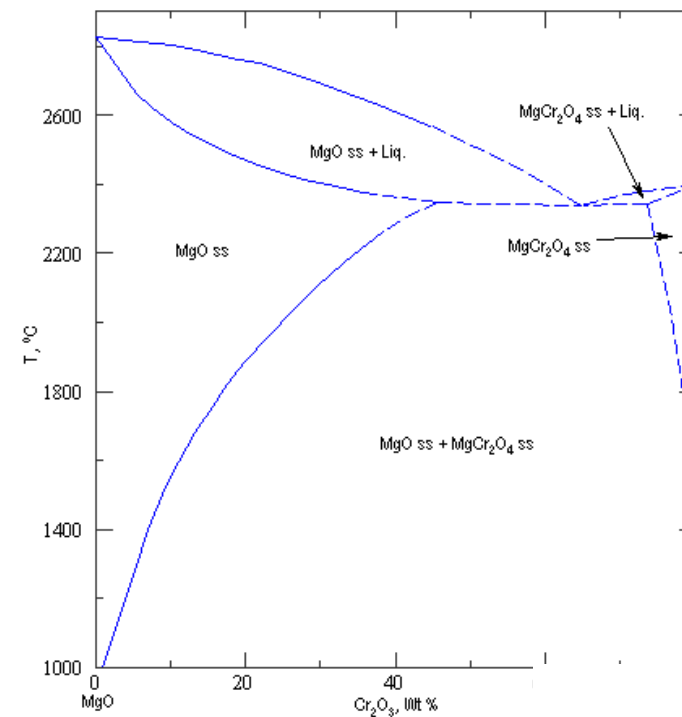


Chromium in EAF slag

EAF 1 (Carbon steel) MgO saturated
EAF 2 (Stainless) not MgO saturated

EAF 1

Cr will be enriched in MgO (ss) instead of forming spinel primary. MgO (ss) can dissolve up to ~ 40 wt%

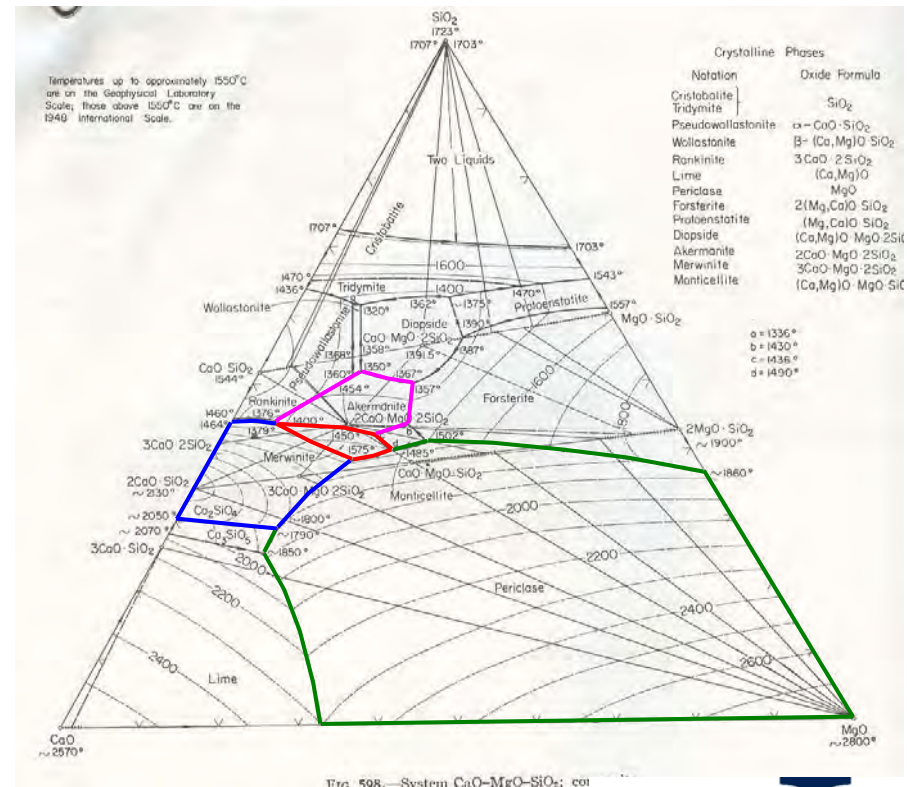


Distribution of chromium

Dissolves chromium

Merwinite	Yes
Akermanite	No
γ - Ca_2SiO_4	No
MgO	Yes
Gehlenit	No
$\text{Ca}_2\text{Fe}_2\text{O}_5$	Yes
$3\text{CaO} \cdot \text{Al}_2\text{O}_3$	No

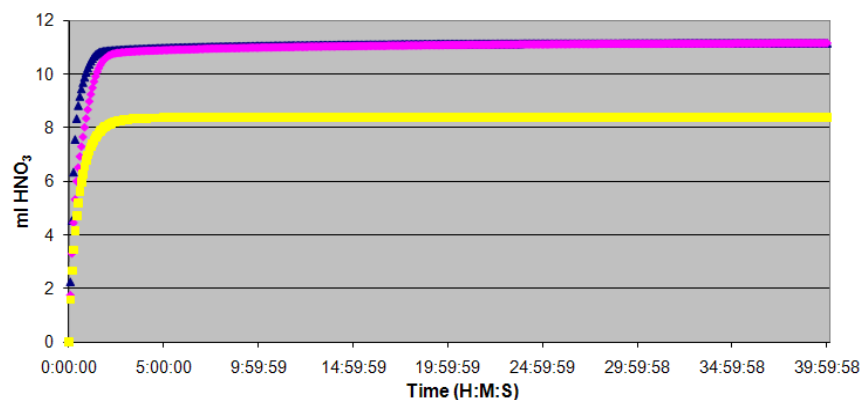
Totally 11 Cr containing slag minerals was found!



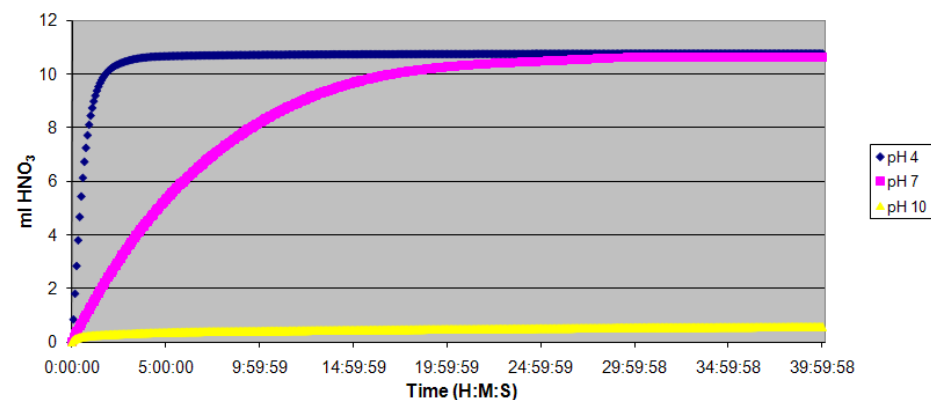
Synthetic slag minerals/titration

20-38 μm size fraction, 0.1 M HNO_3 , 50 mg mineral / 100 ml H_2O

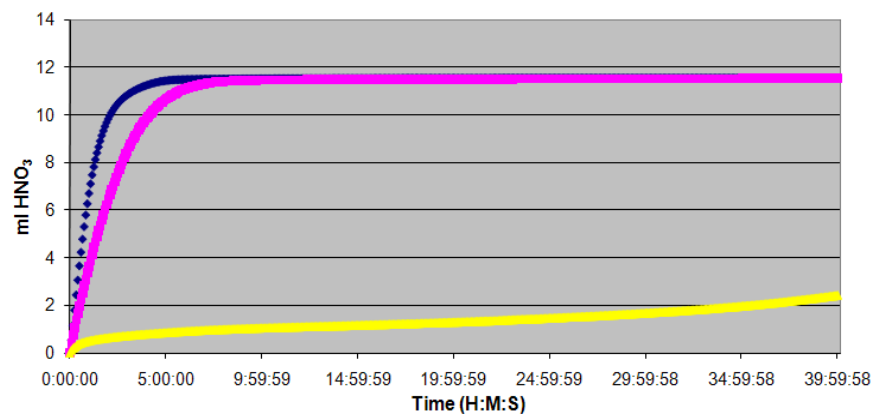
γ -dicalcium silicate (Ca_2SiO_4)



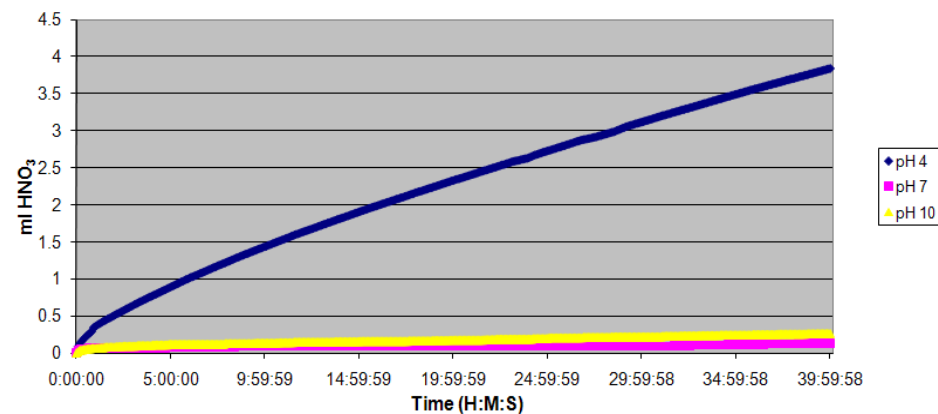
Akermanite ($\text{Ca}_2\text{MgSi}_2\text{O}_7$)



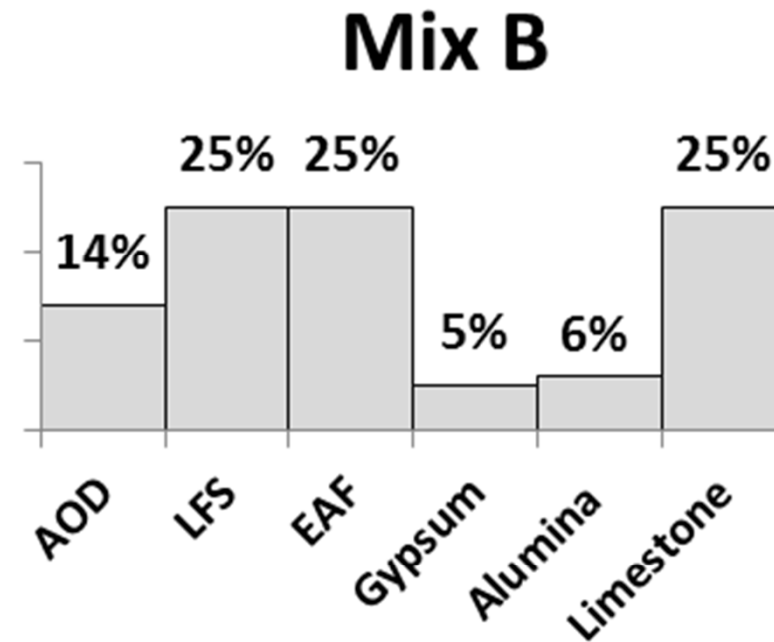
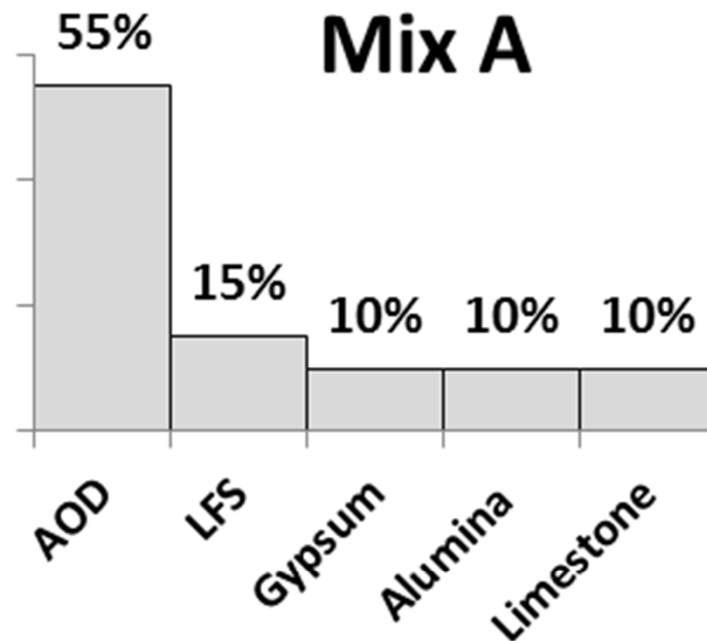
Merwinite ($\text{Ca}_3\text{MgSi}_2\text{O}_8$)



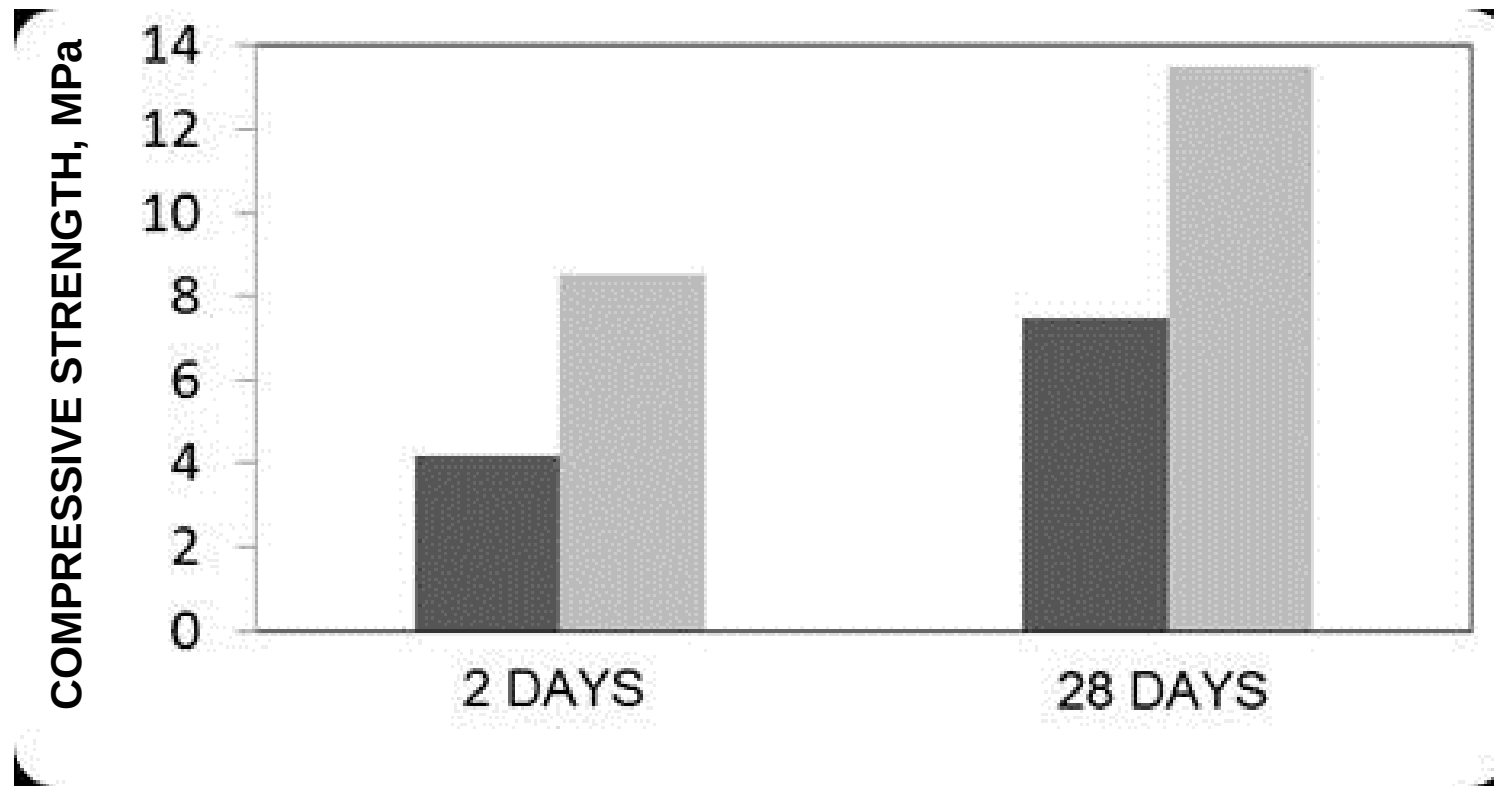
Gehlenite ($\text{Ca}_2\text{Al}_2\text{SiO}_7$)



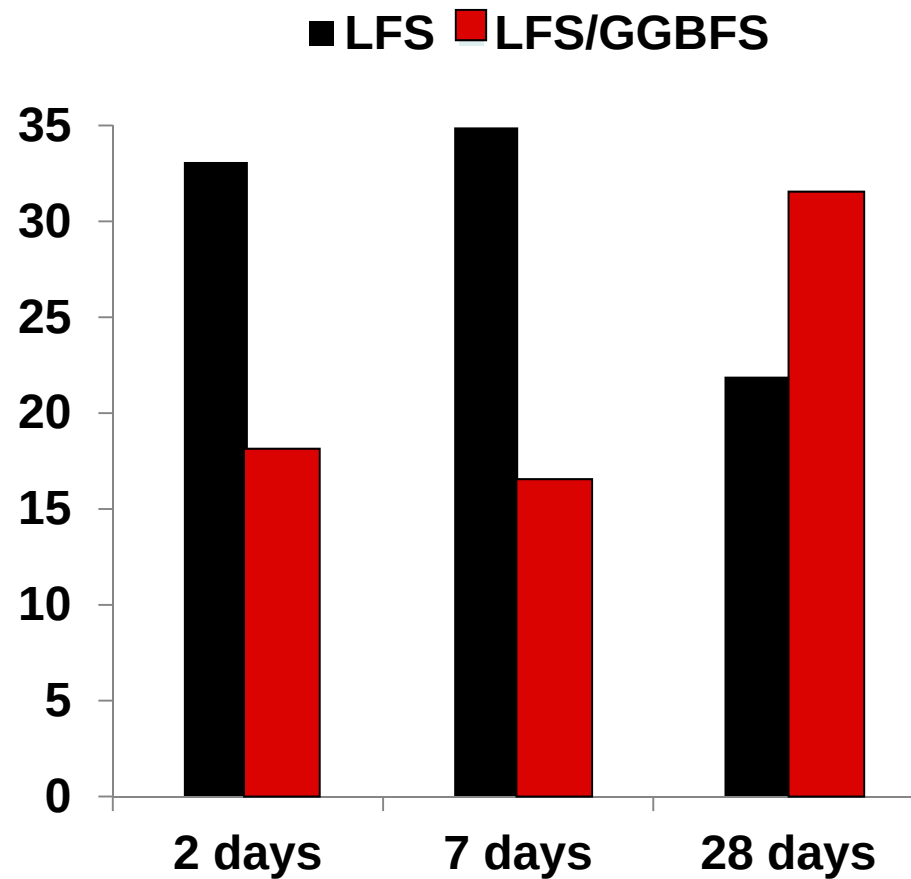
Use of steelmaking slag in production of a SAB-type cement



One mixture containing BOF slag and one with only ladle slag was also tested



Compressive strength for a ladle furnace slag and a mixture with GGBFS





Thanks for listening!

Questions

