# Case Study 9 Ferronickel production

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🐯 McGill CRCT

2013



Ferrous Processing 1

### **Ferronickel production**



After removal of moisture from the laterite, char is added to react with calcined laterite.

**Productions are Slag and Alloys(Fe-Ni).** 

After the calcination, the temperature of laterite is assumed as 500°C Char is assumed to be added at 100°C in the EAF and react at 1600°C

We are considering gas, slag and Fe-alloys in this case study.



Ferrous Processing 2



# Determine the amount of reductant needed to produce Fe-Ni with 25% nickel Composition Target



**Ferrous Processing 3** 

**McGill CRCT** 

#### **Reactants Window**

Reactants - Equilib													
ile Edit Table Units Da	ita Search Help												
🗅 🗃 🕂 🏢 T(C) P(atm) Energy(J) Mass(g) Vol(litre) 👖 🗐 💽 😿													
1.10 11 14													
1 - 10   11 - 14													
Mass(g)	Species	Phase	T(C)	P(total)**	Stream#	Data							
8,1	FeO	solid-FactPS wustite 💌	500	1	1	FactPS							
+ 20,9	Fe203	solid-1-FT oxid hematit 💌	500	1	1	Toxid							
+ 43.8	Si02	solid-1-FT oxid quartz(I 💌	500	1	1	Toxid							
+ 6.4	AI203	solid-4-FT oxid corund 💌	500	1	1	Toxid							
+ 16.8	MgO	solid-FT oxid periclase 💌	500	1	1	Toxid							
+ 2.3	NiO	solid-FT oxid 💌	500	1	1	Toxid							
+ <4.8A>	AI203	solid-4-FT oxid corund 💌	100	1	2	Toxid							
+ <14A>	Si02	solid-1-FT oxid quartz(I 💌	100	1	2	Toxid							
+ <81.2A>	Al2O3: Mol. Wt. =	<mark>101.9612772</mark> β graphit <b>▼</b>	100	1	2	FactPS							
+ 0.1	CaO	solid-FToxid lime 💌	500	1	1	Toxid							
					Initial Conditi	ons							
		Next >>											
ctSage 6.3 Compound:	3/19 databases Soluti	on: 2/19 databases											



Ferrous Processing 4

WCGill CRCT Montreal 2013

#### **Data Search**

q	Data Search				8 L.L.		×
	-Databases -	3/19 compour	nd databases, 2	/19 solution data	bases ———		
	Gact	GactSage"	SGTE	compounds only	ous		
	✓ FactPS			solutions only		🗌 SGTE#	🗆 SGTE*
	✓ FToxid	FSIead FSIite					
		FSstel	SGnobl	Clear All			
	FThall	FSnobl	SGsold	Select All			
				Add/Remove Data	-		
	Fineig	ELEM	Other		1		
	FTlite	FT demo	Direction TDnucl	RefreshDatabases			
	Information Click on a box t compound and (note, this is NC	- to include (or excl solution databasi )T recommended	ude) a database ir e (when available) ).	n the data search. No will be selected. To	rmally databases a 'uncouple' a datab	re 'coupled' - tha ases click-mouse	t is both the eright-button
	If database is s	tored on your PC	but not listed here	then you must 'add th	ne database to the	list' - click on 'Ad	id/Remove'.
	0-6						
	options		de gaseous ions (plas	emas)	Limits	u⊔u ⊻(movi) –	
	Default		aqueous species		organic species C> Minimum solution o	omponents: ∩ 1	2 • 2 cots
			limited data compo	ounds (25C)			
	Canc	el		Summary			ОК



**Ferrous Processing 5** 

**McGill CRCT** 

### Menu Window - Laterite + Char at 1600°C

存 Menu - Equilib: comments	14			
<u>F</u> ile <u>U</u> nits <u>P</u> arameters <u>H</u> elp				
	T(C) P(atm) Energy(J) Ma	ss(g) Vol(litre)	🚻 📑 🔁	
Reactants         [14]           (gram)         20.9         Fe         +         8.1           (500C,s2-FSstel,#1)         (500C,s1	Fe2D3 + 43.8 SiD2 -FToxid,#1) (500C,s1-FToxid,#1)	+ 6.4 Al2O3 + 1 (500C,s4-FT oxid,#1) (5000	16.8 MgO + IC,s-FToxid,#1) (50 ▶	
Froducts     Compound species			Solutions	
★ gas  ideal  real 51     aqueou		Full Name	activities solutions Selection of Gas phases	
pure lique Gas 0 ★ pure solids 116	+ FSstel-FCC1 + FSstel-BCC1	Selection - Equilib - no results -	ity coefficients	٤
suppress duplicates apply * - custom selection	I FToxid-SLAGA ASIa	File Edit Show Sort	sales selected.	
species: 167	I FToxid-MeO_A		- no results -	
	+ FToxid-cPyrA A	Code Species D	Data Phase T V Activity Minimum Maximum	-
Composition target Element Ni - FSstel-LIQU Estimate ALPHA: 1 Mass(g): 0	Legend I - immiscible 4 C - composition target - element: Ni	1         U2(g)         FS           2         Al(g)         FS           +         3         C(g)         Fail           +         4         C2(g)         Fail           +         5         C3(g)         Fail           +         6         C4(g)         Fail	istel g g la	
		+ 7 C5(g) Far	actPS gas	
A>     A>     A>     A>	T(C) P(atm) 1600 1	+         9         02(g)         Far           +         9         02(g)         Far           +         10         03(g)         Far           +         11         CO(g)         Far	actPS gas actPS	
10 steps Table		+ 12 C20(g) Fai + 13 C02(g) Fai + 14 C302(g) Fai	actPS gas actPS gas actPS gas	-
FactSage 6.3 C:\\Equ	uiReactor_Composition_Targe-10Ni-No1-	Show Selected Se	elect All Select/Clear Clear OK	



Ferrous Processing 6

**McGill CRCT** 

### Menu Window - Laterite + Char at 1600°C

File Units Parameters Help							
	T(C) P(atm) Energy	(J) Mass(g) Vol(litre)		👖 🞐 🕒 😿			
Reactants [14] (gram) 20.9 Fe + 8.1 F (500C,s2-FSstel,#1) (500C,s1-1	Fe2O3 + 43.8 SiO; FToxid,#1) (500C,s1-FTox	2 + 6.4 / id,#1) (500C,s4-i	Al2O3 + 16. FToxid,#1) (500C,s	8 MgO + -FToxid,#1) (50			
Products	- Solution species		Custom Solu	tions			
★		Full Name Liquid	O fixed act     O ideal sol     O activity o	ivities utions coefficients	lection o	f Solid p	hases
* + pure solids 116	+ FSstel-BCC1	BCC_	ection - Equilib - no resul	D-1-3- ts -			
* suppress duplicates apply * Pure solids 167	I FToxid-SLAGA I FToxid-SPINA I FToxid-Me0_A	ASlag-liq all ¢ File ASpir AMono Selecte	Edit Show Sort	Duplicates selected.	no results -		
	+ Floxid-cPyrA + FToxid-oPyr	Orthopyr	Code Species	Data Phase	T V Activity	Minimum	Maximum
Composition target Element Ni - FSstel-LIQU Estimate ALPHA: 1 Mass(g): 0	Legend I - immiscible 4 C - composition target - element: Ni	Show C all ( + species: 41 + solutions: 1( + +	220         MnNi3(s)           221         Na2D(s)           222         Na2D(s2)           223         Na2D(s3)           224         MgD(s)           225         Al2D3(s)	FSstel mnni3_mnni3 FToxid solid-a FToxid solid-b FToxid solid-c FToxid periclase FToxid gamma	V		
Final Conditions	T(C) P(atm)		226         Al2U3(\$2)           227         Al2D3(\$3)           228         Al2U3(\$4)           229         NaAID2(\$)           230         NaAID2(\$2)	FToxid deita FToxid kappa FToxid corundum(alpha FToxid solid-a FToxid solid-b	5 V		
10 steps 🗖 Table		1 c + + +	231         NaAl9014(s)           232         Na2Al12019(s)           233         Si02(s)	FToxid beta-alumina FToxid beta2-alumina FToxid quartz(I)	V		
actSage 6.3 C:\\Equ	iReactor_Composition_Targe-10	Ni-No1-a.DAT	Show Selected	Select All Se	elect/Clear	Clear	ОК



Ferrous Processing 7

**McGill CRCT** 

### Menu Window - Laterite + Char at 1600°C

Menu - Equilib: comments	14	
<u>File Units Parameters H</u> elp		
	T(C) P(atm) Energy(J) Mass(g) Vol(litre)	👖 📑 🔁 😿
Reactants         [14]           (gram)         20.9         Fe         +         8.1           (500C,s2-FSstel,#1)         (500C,s1	Fe2O3 + 43.8 SiO2 + 6.4 Al2O3 + -FToxid,#1) (500C,s1-FToxid,#1) (500C,s4-FToxid,#1)	16.8 MgO + (500C,s-FToxid,#1) (500
Products		
Compound species		stom Solutions
* + gas (* local (* lo	C     Fase-Phase     Full Name     ▲     0       C     FSstel-LIQU     LIQUID     0       +     FSstel-FCC1     FCC_A1       +     FSstel-BCC1     BCC_A2	ideal solutions activity coefficients
* - custom selection species: 167	I     FToxid-SENA     Astagrid all oxides + 3       I     FToxid-SPINA     ASpinel       I     FToxid-Me0_A     AMonoxide       +     FToxid-cPyrA     AClinopyroxene	eudonyms bly  List
Composition target Element Ni - FSstel-LIQU	Legend I - immiscible 4 I -	<u>al Species (max 1500)</u> 584 al Solutions (max 40) 16
Estimate ALPHA: 1 Mass(g): 0	Selection of solutions	Default
Final Conditions	Equilib	rium
<a> <b></b></a>	T(C)         P(atm)         ▼         Delta H(J)         ▼         © norma           1600         1         C transi         C transi	al C normal + transitions
10 steps 🗖 Table	1 calculation	Calculate >>
FactSage 6.3 C:\\Eq	uiReactor_Composition_Targe-10Ni-No1-a.DAT	



Ferrous Processing 8

**McGill CRCT** 

### Menu Window – Composition Target

	🗘 Menu - Equilib: comments	14	
	<u>File Units Parameters H</u> elp		
		T(C) P(atm) Energy(J) Mass(g) Vol(litre)	11 🖳 🕞
	Beactants (14)	Composition Target	×
	Solution FSstel-LIQU	+ 43.8 SiO2 #1) (500C,s1-FToxid,# Solution ST53	LIQU Species
✓	<ul> <li>- clear</li> <li>- all species</li> <li>* - custom select species</li> <li>m - merge dilute solution from</li> </ul>	C       species composition         on species       C         Image: species composition       Image: species composition         Image: species composition       Image: species compositition         Image: species composition	Code numbers (568-586) Fe, C, Co, 568 Fe 💌
✓	<ul> <li>solution properties</li> <li>single phase</li> <li>possible 2-phase immiscibility</li> <li>possible 3-phase immiscibility</li> </ul>	+       FSstel-FCC1         +       FSstel-FCC1         +       FSstel-BCC1         I       FToxid-SLAGA         I       FToxid-SPINA         I       FToxid-MeD_A         +       FToxid-CPyrA         +       FToxid-CPyrA	Element ments C O Mg Al Si Ca Cr Mn Fe Co N Element: Ni 🗨
<ul> <li>✓</li> </ul>	<ul> <li>standard stable phase</li> <li>dormant (metastable) phase</li> <li>f - formation target phase</li> <li>P - precipitate target phase</li> <li>S - Scheil cooling target phase</li> <li>D - soliDification calculation</li> <li>C - composition target</li> </ul>	nd miscible 4 proposition target ment: Ni T(C) P(atm) 1 Nore (removes targets)* Values Enter a single value - or enter a Element Ni [0.25] mass fraction: (25%)	a range of values 'first last step'
	Help FactSage 6.3 C:\\EquiReact	Cancel He	elp OK



**Ferrous Processing 9** 

**McGill CRCT** 

### Results Window - Laterite + Char at 1600°C

Results - Equilib 1600 C A=0.038	1	
Output Edit Show Pages		
	T(C) P(atm) Energy(J) Mass(g) Vol(litre)	11 💷 🖻 😿
		FactSage 6.3 🔺
(gram) 8.1 FeO + 20.9 Fe2	03 + 43.8 SiO2 + 6.4 Al2O3 +	
(500,1,s-FactPS,#1) (500,	1,s1-FToxid,#1) (500,1,s1-FToxid,#1) (500	,1,s4-FTox
(gram) 16.8 MgO + 2.3 NiC	) + <4.8A> Al2O3 + <14A> SiO2 +	
(500,1,s-FToxid,#1) (500,	1,s-FToxid,#1) (100,1,s4-FToxid,#2) (100,	1,s1-FToxi
(gram) <81.2A> C + 0.1 Ca	$0 + 0.1 C_0 0 + 0.8 Cr203 +$	
(100,1,s1-FactPS,#2) (500	,1,s-FToxid,#1) (500,1,s-FToxid,#1) (500,	1,s-FToxid
(gram) 0.6 MnO2 + 0.3 Na2	0 =	
(500,1,s-FToxid,#1) (500,	1,s1-FToxid,#1)	
0.05750	-1	
0.25/52 moi gas_ide	al 1 20 502 litro 1 06025-04 gram(am2)	
(7.3500 gram, 0.25752 mc	== 1 0000)	
(1000 0, 1 atm,	C0	FactPS
+ 4 4912E-02	C02	FactPS
+ 6.1427E-05	Fe	FactPS
+ 3.8497E-05	Na	FactPS
+ 2.1527E-05	SiO	FactPS
+ 6.9777E-06	Ni	FactPS
+ 1.2003E-06	Mg	FactPS
+ 5.0642E-07	Mn	FactPS
+ 2.3065E-07	Co	FactPS
+ 1.6261E-07	FeO	FactPS
+ 1.0555E-07	Cr	FactPS
+ 3.7393E-08	SiO2	FactPS
+ 1.9781E-08	CrO	FactPS
+ 4.5947E-09	0	FactPS
+ 3.0436E-09	Cr02	FactPS
+ 1.4467E-09	NiO	FactPS
+ 3.8185E-10	02	FactPS

Laterite 100 g vs Char 0.0381 g Laterite 1 ton vs Char 0.381 kg



Ferrous Processing 10

**McGill CRCT** 

存 Menu - Equilib: change of Ni w	th adding Char		
File Units Parameters Help			
	T(C) P(atm) Energy(J) №	Mass(g) Vol(litre)	🚻 📑 🐨
Reactants         [14]           (gram) 8.1         Fe0         +         20.9           (500C,s-FactPS,#1)         (500C,s <sup>-1</sup>	Fe2D3 + 43.8 SiO2 -FToxid,#1) (500C,s1-FToxid,#1	+ 6.4 Al2O3 ) (500C,s4-FToxid,#1)	+ 16.8 MgD + (500C,s-FToxid,#1) (50
Products			
Compound species	Solution species	Full Name	Custom Solutions
aqueous 0	+ FSstel-LIQU + FSstel-FCC1	LIQUID FCC_A1	0 ideal solutions 0 activity coefficients
★ + pure solids 116     ✓ suppress duplicates apply	+ FSstel-BCC1 I FToxid-SLAGA A	BCC_A2	- Pseudonyms
* - custom selection species: 167	I FToxid-SPINA	ASpinel AMonoxide	apply 🗌 List
Tarad	+ FToxid-cPyrA + FToxid-oPyr	Orthopyroxene	Total Species (max 1500) 584
- none - Estimate ALPHA: 1	Legend I - immiscible 4 + - selected 8 spe	w Call 💿 selected	Total Solutions (max 40) 16
Mass(g): 0	solu	tions: 16 Select	Default
Final Conditions <a> <b>           0 0.1 0.005</b></a>	T(C) P(atm) -	Delta H(J)	arilibrium formal C normal + transitions ransitions only
10 steps Table		21 calculations	pen Calculate >>
FactSage 6.3 C:\\Ec	uiNo6-Fe-Ni_effect_on_Co_and_Cr_c	omposition.DAT	

### Change of Char from 0 to 0.1g based on 100g Laterite Laterite 1 ton vs change of Char from 0 to 1 kg



Ferrous Processing 11

WCGill CRCT Montreal 2013

Output Edit Show Pages         Save or Print       T(C) P(atm) Energy(J) Mass(g) Vol(litre)         Plot       Plot Results         Plot       Plot Results         Equilib Results file       Repeat Plot - gram vs Alpha       =0.045       A=0.05       A=0.055         Stream File       PactSage 6.3       Plot Results Processor: C:\FactSage\Equilot.res       FactSage 6.3       Plot Results Processor: C:\FactSage\Equilot.res         Fact-XML       Fact-XML       Plot Result Plot - gram vs Alpha       Repeat Plot - gram vs Alpha       Plot A=0.05       A=0.05	
Save or Print       T(C) P(atm) Energy(J) Mass(g) Vol(litre)         Plot       Plot Results         Equilib Results file       Repeat Plot - gram vs Alpha       0.045   A=0.05   A=0.055           Stream File       Plot Asset Plot - gram vs Alpha       0.045   A=0.05   A=0.055           Format       D3 + 43.8 Sit Results Processor: C:\FactSage\Equilo.res         Fact-XML       Plot Asset Plot - gram vs Alpha       0.045   A=0.05   A=0.055	
Plot       Plot Results         Equilib Results file       Repeat Plot - gram vs Alpha         Stream File       Repeat Plot - gram vs Alpha         Format       D3 + 43.8 Siter Results Processor: C:\FactSage\Equilo.res         Fact-XML       -3 + 43.8 Siter Results Processor: C:\FactSage\Equilo.res         Fact-XML       -3 + 43.8 Siter Results Processor: C:\FactSage\Equilo.res	
Equilib Results file       Repeat Plot - gram vs Alpha       =0.045       A=0.05       A=0.055         Stream File       Fact Sage 6.3       A=0.05       A=0.055       A=0.055         Format       D3 + 43.8 Site Results Processor: C:\FactSage\Equi0.res       Fact Sage 6.3       A=0.055         Fact-XML       File       Help       A=0.055       A=0.055         Action Act	
Stream File       FactSage 6.3         Format       D3 + 43.8 Sit Results Processor: C:\FactSage\Equi0.res         Fact-XML       + <4.8A> A1; File         Help       + <4.8A> A1; File         Help       + <4.8A> A1; File         Help       + <4.8A> A1; File	
Format       D3 + 43.8 Sit Results Processor: C:\FactSage\Equi0.res         Fact-XML       D3 + 43.8 Sit Results Processor: C:\FactSage\Equi0.res         Fact-XML       + <4.8A> A1; File Help         1, s=FToxid, #1       81 FeD + 20 9 Fe2D3 + 438 SiD2 + 64 Al2D3 +	
Format         1, s1-FToxid, #           Fact-XML         + <4.8A> A1         File         Help           1, s-FToxid, #1         81 Fe0 + 20.9 Fe203 + 438 Si02 + 6.4 Al203 +         •	1
Fact-XML + <4.8A> A1; File Help 1, s=FToxid, #1 81 Fe0 + 20.9 Fe203 + 43.8 Si02 + 6.4 A203 +	1
-, 3 - FIOXIG, +1	
b + 0.1 CoO	4
Fact-Optimal , 1, s-FToxid, #: Axes Variables Minimum	Maximum
D = activity 0	104.58
Fact-Function-Builder Fl,s1-FToxid,# mole 0	2.5887
mole fract. O	0.999983
Kerresn B1 gram O	99.429
(0.77004 gram, 2.40005 02 mb1, 3.7020 weight % ()	99.998
(1600 C, 1 atm, a=1:0000) Alpha 0	0.1
+ 2 3510E-04 0	1600.
Axes: weight % vs Alpha 1.	1.
Delta Cp(J) 19.62	82.696
Y-variable X-variable Swap Axes Delta G(J) -3.8924E+05	-2.7358E+05
Vol(litre) 0	0
- Y-avis Delta H(J) 1.7769E+05	3.1154E+05
Delta V(litr 3.702	101.96
Weight %     Alpha     Delta S(J)     152.43	277.68
• page • 1.	21.
maximum 100 maximum 0.1	
minimum 0 minimum 0 Display	
	🔲 full screen
tick every 5 tick every 0.01 Select Select	s 🔿 Viewer
· · · · · · · · · · · · · · · · · · ·	: 💽 Figure
C integer #	
Axes Select species and phases to be plotted.	Plot >>
Cancel Befresh	
FactSage 6.3 C:\FactSage\Equi0.res 6F	reb13 21 sets

# **Gact**Sage<sup>™</sup>

#### Ferrous Processing 12

**McGill CRCT** 

	Select								
#	Species	Gram (min)	Gram (max)	Wt.%	(min)	₩t.% (max)	Activity (min)	Activity (max)	
48	Cola	5.6271E-11	4.5397E-06	7.3018E	E-09	8.9375E-05	3.9645E-11	4.5347E-07	
49	Nila	2.4118E-08	2.3166E-04	3.12968	E-06	5.3523E-03	1.7062E-08	3.2792E-05	
50	NiO(a)	2.0065E-10	1.1828E-06	1.07828	E-09	4.2251E-05	4.0498E-12	2.3422E-07	
51	Ni(CO)4(a)	0	1.5441E-15	0		3.0551E-14	0	5.3505E-17	
FSste	I- LIQU								
52	Fe(LIQU)	0	20.715	2.225	Results	Processor: C:\FactS	age\Equi0.res		
53	C(LIQU)	0	0.172327	0 -	ila Llala				
54	Co(LIQU)	0	7.8630E-02	0.214	пе негр				
55	Cr(LIQU)	0	0.384669	3.429		8.1 Fe0	) + 20.9 Fe2O3 + 43.	8 SiO2 + 6.4 Al2O3 +	•
56	AI(LIQU)	0	5.1829E-05	2.307	Axes	Variable		Minimum	Maximum
57	Mn(LIQU)	0	3.8302E-02	4.711		acti	vity	0	104.58
58	Ni(LIQU)	0	1.8073	7.319		ſſ	ole	0	2.5887
59	SI(LIQU)	0	1.4944	1.375		mole fr	act.	0	0.999983
60	Mg(LIQU)	0	9.3987E-07	6.518		g	am	0	99.429
61	O(LIQU)	0	9.6386E-03	4.271		weigh	lt %	0	99.998
62	AIO(LIQU)	0	1.6660E-06	3.131		Al	oha	0	0.1
63	AI20(LIQU)	0	1.4529E-09	2.600				1600.	1600.
64	CrO(LIQU)	0	3.5027E-04	3.473		Pla Dalha C	itmj - CD	10.00	l. 03.000
						Deita C Deita (	P(J) S(D) -	13.02 3.892/F±05	-2 7358E±05
			—	s –		Vol(	tre)	0	- <u></u>
				nole		Delta I	101	1.7769E+05	3.1154E+05
			🗆 [page] 🖉 🧿	Iram		Delta \	/(litr	3.702	101.96
CL						Delta	6(J)	152.43	277.68
			21 pages			- paj	je -	1.	21.
Click on t	he '+' column to add (	or remove species.		F	Axes	Species	Grap	h Disp	lau
					0 selec	oted O sele	cted Labe		olor 🗌 full ser
						Cal	size	: 9 no: 4 🔽 r	eactants 🕜 Viewei
						Seit	· · · · ·	shemical 🛛 🔽 fi	ile name 🛛 📀 Figure
							O i	nteger #	
					Axe	<sup>S</sup> Select species an	d phases to be plotte	ed. ₹	Plot >>



Ferrous Processing 13





With addition of Change the contents of Ni dissolved in liquid iron decrease. If then, what are amounts of Fe-Ni and Slag after each process?



Ferrous Processing 14

🐯 McGill CRCT

Montreal

Results - Equilib A=0 (page 1/2	1)				<b>X</b>	
Output Edit Show Pages Save or Print	T(C) P(atm	atm) Energy(J) Mass(g) Vol(litre) 👖 📑 🐺				
Plot	Plot Results					
Equilib Results file	Repeat Plot -	gram vs Alj	pha =0.04	45 A=0.05 A=0.055		
Stream File Format	D3 + 43.8 Si 1,s1-FToxid,#	Results Pro	ocessor: C:\FactSage\Equi0	FactSage 6	x	
Fact-XML	+ <4.8A> A1; <sup>F</sup> 1,s-FToxid,#1 0 + 0.1 Co0	lie Help	8.1 FeO + 20.9 Fe	e2O3 + 43.8 SiO2 + 6.4 Al2O3	+ 🔽	
Fact-Optimal	,1,s-FToxid,#:	Axes	Variables	Minimum	Maximum	
	D =		activity	0	104.58	
Fact-Function-Builder	1,s1-FToxid,#1		mole	0	2.5887	
Defeash			mole fract.	0	0.999983	
Refresh	B1 R mol 2 7020		gram	0	99.429	
(1600 C 1 atm	a=1 0000)		weight %	U	99.998	
(0,99973	02		Alpha	U 1000	U.1	
+ 2.3510E-04	0		D(also)	1600.	1600.	
Axes: gram vs Alpha			E Collina Coll	1962	02.000	
			Deita Op(i)	-3.8924E±05	-2 73585+05	
variable X-variable Swap Axes			Vol(litre)	-3.03246+03	0	
			Delta H(J)	1 7769E+05	3 1154E+05	
-Y-axis X-axis			Delta V(litr	3 702	101.96	
gram Alpha			Delta S(J)	152.43	277.68	
			- page -	1.	21.	
maximum 100 maximum 0.1 minimum 0 tick every 5 tick every 0.01		Axes O selected Axes	d Select Select species and phases t	Graph Labels size: 9 no: 4 ♥ ♥ C chemical ♥ o be plotted. ₽	play color ☐ full screen reactants C Viewer file name	
Cancel Refresh	OK Fa	actSage 6.3	C:\FactSage\Equi0.res		6Feb13 21 sets	



#### Ferrous Processing 15



7	Species Se	election - EQUILIB	Results: gram vs A	Alpha			840	-		×	
File	Show	Select									
	· #	Species	Gram (min)	Gram (m	ax) V	√t.% (min)	₩t.% (max)	Activity (min)	Activity (max		
		SOLUTIONS									
	585	GAS	0.770643	18.611	0	)	0	1.	1.		
+	586	LIQU	0	24.691	0	)	0	3.9934E-03	1.		
-	587	FLLT	0	0	0	)	n	A 2980E-04	0.947531		
	588	BCC1	0	0	0	🍞 Results I	Processor: C:\FactSage	e\Equi0.res			×
+	589	SLAGA#1	66.898	99.429	0	File Heln					
	590	SLAGA#2	0	0	0						
	591	SPINA#1	0	0	0		8.1 FeO +	20.9 Fe2O3 + 43.8 S	i02 + 6.4 Al203 +	-	
	592	SPINA#2	0	0	0	Axes	Variables	Mi	nimum		4 aximum
	593	MeO_A#1	0	0	0		activity	,	0		104.58
	594	MeO_A#2	0	0	0		mole	•	0		2.5887
	595	сРугА	0	0	0		mole fract.		0		0.999983
	596	oPyr	0	0	0		gram	1	0		99.429
	597	pPyrA	0	0	0		weight %	:	0		99.998
	598	OlivA	0	0	0		Alpha	1	0		0.1
	599	MulF	0	0	0		T(C)	1	600. ·		1600.
	600	CORU#1	0	0	0		P(atm)		l.		1.
	601	CORU#2	0	0	0		Delta Up(J)		3.62 0045.05		82.696
_							Deita G(J) Volfikoj	) -3.8 )	0 0	-2	0
							Vol(iitie) Delta H(I)	17	0 769E±05		1154E±05
				source	Mass O mole		Delta V(litr	, i.i	702		101.96
							Delta S(J)	1!	52.43		277.68
				[[hage]	is gram		- page -		I.		21.
	Clea	ſ		21 pages		- Avae	Species	Granh			
Click on the '+' column to add or remove species.						O selec	ted 0 selecte			lay olor	full screen
							Select	size:  5         G che         Citate	mical fi	eactants le name	<ul> <li>Viewer</li> <li>Figure</li> </ul>
						Axe	Select species and p	hases to be plotted.	) }	Plo	it >>
						FactSage 6.3	3 C:\FactSage\Eq	ui0.res		6Feb1	13 21 sets



Ferrous Processing 16

**McGill CRCT** 





Ferrous Processing 17

WCGill CRCT Montreal





Ferrous Processing 18



# Determine the liquidus temperatures of slag and alloy (Fe-25wt% Ni)

Stream / Precipitate Target



**Ferrous Processing 19** 

The Gill CRCT

### Liquidus Temp. of Alloy – Creating Stream file

4	Results - Equilib 1600 C, A=0.	0015					x
<u>0</u> u	t <b>put</b> <u>E</u> dit <u>S</u> how Pages						
	Save or Print Plot	;	T(C) P(atm) Energy(J) Mass(g) '	Vol(litre)		111 🖳 🖻	
	Equilib Results file	٠t			F	actSage 6.	3 🔺
	Stream File	•	Recycle all streams				
	Format	•	Save stream file	•	Save gas phase		
	Fact-XML	•	Stream file properties		Save pure liquids		
	Fact-Optimal	•	Summary of streams	•	Save aqueous Save pure solids		
	Fact-Function-Builder	•	Directory (C:\FactSage\)	_	Save solutions	• •	ALL solutions
	Refresh	3	mol, 1.3989 litre, 1.8501E-	04 gra	m/cm3)		FSstel-LIQU LIQUID
T	( 0.97332	_	co		FactPS		FSstel-FCC1 FCC_A1
	+ 2.6511E-02		C02		FactPS		FSstel-BCC1 BCC_A2
	+ 7.4349E-05 + 4.6063E-05		re Na		FactPS		FToxid-SLAGA#1 ASlag-liq
	+ 4.2801E-05		SiO		FactPS		FToxid-SLAGA#2 ASlag-lig
	+ 2.6804E-06		Ni		FactPS		ETavid SDINA#1 ASsignal
	+ 2.0202E-06		Mg		FactPS		FT0xid-SPINA#1 ASpiner
	+ 8.5857E-07 + 2.0347E-07		Mn Cr		FactPS		FToxid-SPINA#2 ASpinel
	+ 1.1399E-07		FeO		FactPS		FToxid-MeO_A#1 AMonoxide
	+ 8.7497E-08		Co		FactPS		FToxid-MeO A#2 AMonoxide
	+ 4.3057E-08		SiO2		FactPS		
	+ 2.2085E-08		CrO		FactPS		FToxid-cPyrA AClinopyroxene
	+ 1 9679E-09		Cr02		FactPS		FToxid-oPyr Orthopyroxene
	+ 3.2184E-10		NiO		FactPS		FToxid-pPyrA AProtopyroxene
	+ 1.4791E-10		MgO		FactPS		
							FTOXID-UIIVA AUTIVINE
							FToxid-MulF Mullite
							FToxid-CORU#1 M2O3(Corundum)
							FToxid-CORU#2 M2O3(Corundum)



Ferrous Processing 20

**McGill CRCT** 

### Liquidus Temp. of Slag – Creating Stream file

Q	Results - Equilib 1600 C, A=0.	0015					×
<u>0</u>	Itput Edit Show Pages						
	Save or Print Plot	*	T(C) P(atm) Energy(J) Mass(g)	Vol(litre)		111 🖳 🕻	
	Equilib Results file	•			F	actSage 6	.3 .
	Stream File	►	Recycle all streams				
	Format		Save stream file	•	Save gas phase		
	Fact-XML	•	Stream file properties		Save pure liquids		
	Eact Ontimal		Summary of streams	•	Save aqueous		
	ract-optimal	<b>_</b>	Directory (C:\FactSage\)		Save pure solids		
	Fact-Function-Builder	٠h	1	_	Save solutions	+	ALL solutions
	Refresh		3 mol, 1.3989 litre, 1.8501E	-04 gra	m/cm3)		FSstel-LIQU LIQUID
Т	( 0.97332		a=1.0000) CO		FactPS		FSstel-FCC1 FCC_A1
	+ 2.6511E-02		C02		FactPS		FSstel-BCC1 BCC_A2
	+ 7.4349E-05		Fe		FactPS		FToxid-SLAGA#1 ASlag-lig
	+ 4.6063E-05		Na		FactPS		ETavid SLACA#2 ASIan lin
	+ 2.6804E-06		Ni		FactPS		FToxid-SLAGA#2 ASiag-liq
	+ 2.0202E-06		Mg		FactPS		FToxid-SPINA#1 ASpinel
	+ 8.5857E-07		Mn		FactPS		FToxid-SPINA#2 ASpinel
	+ 2.0347E-07		Cr		FactPS		ETavid MaQ A#1 AManavida
	+ 1.1399E-07		FeO		FactPS		FT0xid=meO_A#1 Amonoxide
	+ 4.3057E-08		SiO2		FactPS		FToxid-MeO_A#2 AMonoxide
	+ 2.2085E-08		CrO		FactPS		FToxid-cPyrA AClinopyroxene
	+ 2.6610E-09		0		FactPS		FT ovid-oDyr Orthonyrovene
	+ 1.9679E-09		Cr02		FactPS		r toxid-or yr orthopyroxene
	+ 3.2184E-10		NiO M-O		FactPS		FToxid-pPyrA AProtopyroxene
	+ 1.4/51E-10				FactPS		FToxid-OlivA AOlivine
							EToxid-MulE Mullite
							FT-wid CORU#1 M202/Commenters)
							FToxia-COKU#1 M2O3(Corundum)
							FToxid-CORU#2 M2O3(Corundum)



Ferrous Processing 21

**McGill CRCT** 

### Liquidus Temp. of Alloy – Import Stream file





Ferrous Processing 22

WcGill CRCT Montreal 2013

### Liquidus Temp. of Alloy – Precipitate Target

Q.	Reactant	ts - Equilib							X
<u>F</u> ile	<u>E</u> dit	<u>T</u> able <u>U</u> nits	<u>D</u> ata Search	<u>H</u> elp					
	<b>2</b>	+		T(C) P(atm)	Energy(J) Mass(g)	) Vol(litre)		III 🖳	釆
-									
	1.1								1
				C		T(C)		C1# D-1	
	10	Mass(g)	[FSste	Species	Stream		P(total)-		a
	1.0				Lougan!	1,000	1.		
								Initial Conditions	
					Nout				
					Nex( >>				



**Ferrous Processing 23** 

**McGill CRCT** 

### Liquidus Temp. of Alloy – Precipitate Target

存 Menu - Equilib: Steel Cooling	14	
<u>File Units Parameters Help</u>	T(C) P(atm) Energy(J) Mass(g) Vol(litre)	M 🗩 🖻 😿
	(gram) 100% [FSstel-LIQU_LIQUID] (1600C,liq,#1)	Solution FSstel-LIQU - clear
Products     Compound species     ★ + gas   ideal  real 48     aqueous 0     pure liquids 0     * + pure solids 109     suppres Click mourse-right	Solution species         *       Base-Phase       Full Name         P       FSstel-LIQU       LIQUID         +       FSstel-FCC1       FCC_A1         +       FSstel-BCC1       BCC_A2         buttor       to open Selection Window for ESstel-ECC1	<ul> <li>- all species</li> <li>* - custom select species</li> <li>m - merge dilute solution from</li> <li>- solution properties</li> <li>+ - single phase</li> </ul>
* - custom selection species: 157		<ul> <li>I - possible 2-phase immiscibility</li> <li>J - possible 3-phase immiscibility</li> <li>- standard stable phase</li> </ul>
FSstel-LIQU Estimate T(C): 1000 Mass(g): 0	P - precipitate target + - selected 2 Show ○ all ⓒ selected species: 55 solutions: 3	<ul> <li>! - dormant (metastable) phase</li> <li>F - formation target phase</li> <li>P - precipitate target phase</li> </ul>
Final Conditions <a>       Image: A interval of the steps       10       steps</a>	T(C) P(atm) ▼ Delta H(J) ▼ 1 1 calculation	<ul> <li>S - Scheil cooling target phase</li> <li>D - soliDification calculation</li> <li>C - composition target</li> </ul>
FactSage 6.3 C:\FactS	age\EquiSteel-cooling-No2-b.DAT	Help



Ferrous Processing 24

**McGill CRCT** 

### Liquidus Temp. of Alloy – Precipitate Target

🕞 Results - Equilib 1599.96 C		
Output Edit Show Pages		
	T(C) P(atm) Energy(J) Mass(g) Vol(litre)	M 🖳 🔁 😿
		FactSage 6.3
(1600,1,liq,#1)	-	
0 mol gas_ideal		
(1599.96 C, 1 atm,	a=1.0000)	
( 0.95499 CO	Fa	ctPS
+ 4.4922E-02 CO2	Fa	ctPS
+ 6.1399E-05 Fe	Fa	ctPS
+ 2.1523E-05 SiO	Fa	ctPS
+ 6.9743E-06 Ni	Fa	ctPS
+ 1.2001E-06 Mg	ra T-	etPS
+ 5.062/E-0/ Mn	11 7-	etPS
+ 1 6255E-07 E-0	11 7-	et DS
+ 1.0255E-07 Fe0	11 7-	et DS
+ 3 73907-08 5102	ra Fa	ot DS
+ 1 9775E-08 Cr0		ct DS
+ 4 59268-09 0	Fa	ctPS
+ 3 0432E-09 Cr02	Fa	ctPS
+ 1.4459E-09 NiO	Fa	ctPS
+ 3.8173E-10 O2	Fa	ctPS
+ 1.5170E-10 MgO	Fa	ctPS
+ 1.3795E-12 Cr03	Fa	ctPS
+ 1.0866E-12 Si	Fa	ctPS
+ 8.4551E-13 Al	Fa	ctPS
+ 7.5318E-13 AlO	Fa	ctPS
+ 4.7334E-13 C20	Fa	ctPS
+ 3.4142E-13 Ca	Fa	ctPS
+ 1.7660E-13 C302	Fa	ctPS +
J		



Ferrous Processing 25

**McGill CRCT** 

### Liquidus Temp. of Slag – Import Stream file





Ferrous Processing 26

🐯 McGill CRCT

Montreal

# Liquidus Temp. of Slag – Precipitate Target

<u>File Edit Table Units</u>	<u>D</u> ata Search <u>H</u> elp	
D 🗃 🕂 💷	T(C) P(atm) Energy(J) Mass(g) Vol(litre)	11 📑 📑 🧃
1-1		
Mass(g)	Species Phase T(C)	P(total)** Stream# Data
1100/6		
		Initial Conditions
		,
	Nort >>	
	Next >>	

### Liquidus Temp. of Slag – Precipitate Target

存 Menu - Equilib: Slag cooling	14 1	
File Units Parameters Help	T(C) P(atm) Energy(J) Mass(g) Vol(litre)	
Reactants (1)		Solution FToxid-SLAGA
	(gram) 100% [FToxide_Slag] (1600C,#1)	- clear
Products		* - custom select species
Compound species	- Solution species	m - merge dilute solution from
* ∓ gas ⊙ ideal ⊂ real 34	🕴 + Base-Phase 🛛 Full Name 🔺	solution properties
aqueous 0	IP FToxid-SLAGA ASIaq-lig all oxides + S	- solution properties
pure liquids 0	I FToxid-SPINA ASpinel	L single phase
* + pure solids 114	I FToxid-MeO A AMonoxide	+ - single phase
E suppress duplicates, applu		<ul> <li>I - possible 2-phase immiscibility</li> </ul>
suppress adplicates apply	+ EToxid-oPur Orthopurovene	L - nossible 3-nbase immiscibility
species: 148	+ FT oxid-oPurA AProtopyroxene	y possible y pruse inimiseibility
		- standard stable phase
" * " denotes custom selectio	on - not all the species have been selected.	
- Precipitate Target-		! - dormant (metastable) phase
FToxid-SLAGA	Legend Show C all Selected	F - formation target phase
Estimate T(C): 1000	P - precipitate target	P - precipitate target phase
Manufalt 0	+-selected 2 solutions: 16	
Mass(g). Jo		5 - Schell cooling target phase
- Final Conditions		D - soliDification calculation
	T(C) P(atm) 💌 Delta H(J) 💌	C - composition target
	1	Help
10 steps Table	1 calculation	Calculate >>
FactSage 6.3 C:\FactSag	ge\EquiSlag-cooling-No2-a.DAT	



Ferrous Processing 28

**McGill CRCT** 

### Liquidus Temp. of Slag – Precipitate Target

存 Results - Equilib 1380.48 C			1	
Output Edit Show Pages				
	T(C) P(atm) Energy(J	I) Mass(g) Vol(litre)		11 🖳 🕞 😿
	3.82072-05	7 100CF_05		A
E E	2.73852-03	0 17447		
Mn	1 73208-03	4 23838-03		
Cr	2 62618-03	6 0820E-03		
Ca	4 4773E-04	7 9926E-04		
Si	0.18525	0.23174		
Al	3.2420E-02	3.8963E-02		
Mg	0.10466	0.11330		
Na	2.4281E-03	2.4864E-03		
0	0.60023	0.42775		
+ 0 gram A01 (1380.48 C, (37.233) + 5.1126 + 12.725 + 23.821 + 3.5553E-10 + 1.1064E-03 + 1.6546E-06 + 5.0756E-03 + 4.0547E-06 + 1.4338E-03 + 3.5096E-08 + 1.4617E-05 + 7.6010E-07 + 1.1247E-05 + 9.6934E-05 + 1.1400E-02	<pre>ivine#1 1 atm, a=1.0000) wt.% Mg1Mg1S1104 wt.% Fe1Fe1Si104 wt.% Fe1Mg1Si104 wt.% CalCalSi104 wt.% CalFe1Si104 wt.% CalMg1Si104 wt.% CalMg1Si104 wt.% Mg1CalSi104 wt.% Mn1Mn1Si104 wt.% CalMn1Si104 wt.% ColColSi104 wt.% ColColSi104 wt.% Mn1ColSi104 wt.% Mg1ColSi104 wt.% Mg1ColSi104</pre>		FToxid FToxid FToxid FToxid FToxid FToxid FToxid FToxid FToxid FToxid FToxid FToxid FToxid FToxid	



Ferrous Processing 29

**McGill CRCT** 

# Show the impact of the SiO<sub>2</sub>/MgO (in the range of 1 to 4) ratio on the liquidus temperature of the slag (Primary crystallization phase) Stream / Precipitate Target



Ferrous Processing 30

🐯 McGill CRCT

#### Addition of 0.381 kg of Char with 1 tone of Laterite SiO<sub>2</sub>+MgO = 60.6 wt%

<b>≆</b>   +  <u>m</u>	T(C) P(al	tm) Energy(J) Mass(g) Vol(litre	:)		111 <b>-</b>	🤋 🖻
10   11 - 14						
Mass(g)	Species	Phase	T(C)	P(total)**	Stream#	Data
8,1	FeO	solid-FactPS wustite 💌	500	1	1	FactP9
20,9	Fe203	solid-1-FT oxid hematit 💌	500	1	1	FToxid
<60.6-A>	SiO2	solid-1-FToxid quartz(I 💌	500	1	1	FToxid
6.4	AI203	solid-4-FToxid corund 💌	500	1	1	FToxid
A>	MgO	solid-FToxid periclase 💌	500	1	1	FToxid
2.3	NiO	solid-FT oxid 🗨	500	1	1	FToxid
<4.8B>	AI203	solid-4-FT oxid corund	100	1	2	FToxid
<14B>	Si02	solid-2-FT oxid quartz(ł 💌	100	1	2	FToxid
<81.2B>		solid-1-FactPS_graphit 💌	100	1	2	FactP9
0.1	CaO	solid-FT oxid lime	500	1	1	FToxid
				~	Initial Condi	tions
			_		_	



### **Ferrous Processing 31**

🐯 McGill CRCT

Montreal

# MgO = 12.12 to 30.3 wt% $SiO_2/MgO = 1 \text{ to } 4 \text{ ratio}$

Menu - Equilib: 37 Calculations		
<u>File Units Parameters H</u> elp		
	T(C) P(atm) Energy(J) Mass(g) Vol(litre)	🚻 📑 🐼
Reactants         [14]           <60.6-A>         SiO2         +         6.4 //           (500C,s1-FToxid,#1)         (500C,s4-           ▲	Al2O3 + <a> MgO + 2.3 NiO FToxid,#1) (500C,s-FToxid,#1) (500C,s-FToxid,#1)</a>	+ <4.88> Al2O3 + < (100C,s4-FT oxid,#2) (100(
Products		- Custom Solutions
★ + gas  ideal  real 51     aqueous 0     pure liquids 0     + pure solids 116     suppress duplicates apply     * - custom selection     species: 167     Target     - none -     Estimate T(C): 1000     Mass(g): 0	Image: species       Full Name         Image: species       FSstel-Phase       Full Name         Image: species       FSstel-FCC1       FICC_A1         Image: species       FT oxid-SLAGA       ASlag-liq all oxides + S         Image: species       Image: species       FT oxid-SPINA         Image: species       FT oxid-OPyr       Orthopyroxene         Image: species       41       FT oxid-OPyr         Image: species       417       Select	0 fixed activities 0 ideal solutions 0 activity coefficients Details Pseudonyms apply □ List □ include molar volumes <u>Total Species (max 1500)</u> 584 <u>Total Solutions (max 40)</u> 16
- Final Conditions		quilibrium
A> <b> 12.12 30.3 0.5</b>	I(U)         P(atm)         ▼         Delta H(J)         ▼         ©           1600         1          0<	normal C normal + transitions transitions only
FactSage 6.3	37 calculations	Calculate >>



Ferrous Processing 32

WCGill CRCT Montreal 2013

Results - Equilib A=12.12 (page 1/38)							
Output Edit Show Pages							
D 🖻 🖾 🚮 🗴	T(C) P(atm) Energy(J) Mass(g) Vol(litre)	III 🖳 🔁 😿					
A=24.12							
A=18.12 A=18.62 A=19.12 A=19	.62 A=20.12 A=20.62 A=21.12 A=21.62 A=22.12	A=22.62 A=23.12 A=23.62					
A=12.12 A=12.62 A=13.12 A=13.62 A=14.12 A=14.62 A=15.12 A=15.62 A=16.12 A=16.62 A=17.12 A=17.62							
		FratSam ( 2					
(gram) 20 9 Fe + 8 1 Fe203	+ <60 6-A> SiO2 + 6 4 A12O3 +	ractbage 6.5					
(500.1.s2-FSstel.#1) (500.	1.s1-FToxid.#1) (500.1.s1-FToxid.#1) (500.)	1.94-FT0					
(gram) <a> MgO + 2.3 NiO +</a>	<4.8(0.0015) > A1203 + <14(0.0015) > Si02	+					
(500,1,s-FToxid,#1) (500,1	<pre>s-FToxid,#1) (100,1,s4-FToxid,#2) (100,1,</pre>	s2-FToxi					
(gram) <81.2(0.0015)> C +	0.1 CaO + 0.1 CoO + 0.8 Cr2O3 +						
(100,1,s1-FactPS,#2) (500,	1,s-FToxid,#1) (500,1,s-FToxid,#1) (500,1,	s-FToxid					
(gram) 0.6 MnO2 + 0.3 Na20	=						
(500,1,s-FToxid,#1) (500,1	,s1-FToxid,#1)						
	_						
9.2135E-03 mol gas_idea							
(0.26153 gram, 9.2135E-03	mol, 1.4162 litre, 1.8467E-04 gram/cm3)						
(1600 C, 1 atm,	a=1.0000)	East DC					
( 0.57654 + 2.2204E-02	C0	FactPS					
+ 7 43068-05	Fa	Fact DS					
+ 6 5345E-05	sio	FactDS					
+ 3.1435E-05	Na	FactPS					
+ 2.6810E-06	Ni	FactPS					
+ 1.3820E-06	Mg	FactPS					
+ 8.1622E-07	Mn	FactPS					
+ 2.1625E-07	Cr	FactPS					
+ 9.9725E-08	FeO	FactPS					
+ 8.7642E-08	Co	FactPS					
+ 5.7545E-08	SiO2	FactPS					
+ 2.0547E-08	CrO	FactPS					
+ 2.3294E-09	0	FactPS					
+ 1 6028E-09	Cr02	FactPS					

37 different Slags and Alloys are formed with change of SiO<sub>2</sub>/MgO at 1600°C.

**McGill CRCT** 

Montreal 2013



Ferrous Processing 33

🖓 R	esults - Equilib A=12.12 (pa	e 1/38)	
Out	out <u>E</u> dit <u>S</u> how Pages		
	Save or Print	Save or Print As litre)	111 🖳 🕒 😿
	Plot	Repeat Open Spreadsheet	
	Equilib Results file	▶ 9.62 A=20.12 A=20.62 A=21.12 A=21.62 A=22.12 A=22.62	2 A=23.12 A=23.62
	Stream File	52 A=14.12 A=14.62 A=15.12 A=15.62 A=16.12 A=16.62	A=17.12   A=17.62
	Format	+ <60 6-3> Si02 + 6 4 31203 +	FactSage 6.3 🔺
	Fact-XML	<pre>, 1, s1-FToxid, #1) (500, 1, s1-FToxid, #1) (500, 1, s4-FT + &lt;4.8(0.0015)&gt; Al203 + &lt;14(0.0015)&gt; Si02 +</pre>	.o
	Fact-Optimal	<pre>1,s-FToxid,#1) (100,1,s4-FToxid,#2) (100,1,s2-FTox 0.1 CaO + 0.1 CoO + 0.8 Cr2O3 +</pre>	ri
	Fact-Function-Builder	<pre>,1,s-FToxid,#1) (500,1,s-FToxid,#1) (500,1,s-FToxi ) =</pre>	.d
	Refresh	1,s1-FToxid,#1)	
	9.2135E-03 mol gas_	deal	
	(0.26153 gram, 9.2135	-03 mol, 1.4162 litre, 1.8467E-04 gram/cm3)	
	(1600 C, 1 at ( 0 97654	(, a=1.0000)	,
	+ 2 3284E-02	CO2 Fact PS	
	+ 7.4306E-05	Fe FactPS	
	+ 6.5345E-05	SiO FactPS	5
	+ 3.1435E-05	Na FactPS	3
	+ 2.6810E-06	Ni FactPS	3
	+ 1.3820E-06	Mg FactPS	5
	+ 8.1622E-07	Mn FactPS	5
	+ 2.1625E-07	Cr FactPS	5
	+ 9.9725E-08	FeO FactPS	3
	+ 8.7642E-08	Co FactPS	5
	+ 5.7545E-08	SiO2 FactPS	5
	+ 2.0547E-08	CrO FactPS	5
	+ 2.3294E-09	0 FactPS	-
	+ 1 6028E-09	CrO2 FactPS	·

To export wt% of SiO<sub>2</sub> and MgO in Slag phase



Ferrous Processing 34

WCGill CRCT Montreal 2013

Output	×	🕞 Spi	eadshe	et - Equilib Page	38/38 : T((	c) = 1600, P(atr	n) = 1,	Alpha = 30.3			x
Page Range	Type of Output	File	Edit S	how							
<ul> <li>All 38 pages</li> </ul>	C Printer Printer setup	Select	od: 2/50	2 Spreadshe	ot Species	1		38		- 38 🔽 (pag	el
C Current page 1	◯ Text file (*.txt)		Selected:         2/302         Spreadsheet Species         100         Images         110         110         Images         110         110         110         110         110         110         110         110         110         110         110         110         110         110         1								
	C Equilib Results File (Equi*.res)	+	Code	Species	Data	Phase	τv	Activity	Minimum	Maximum	
			1050	Na2O(SLAGA) Al2O3(SLAGA)	FToxid	FToxid-SLAGA		1.8600E-10 3.3995E-03	1.6164E-12 [1] 2.9345E-04 [3]	1.8600E-10 [38] 3.3995E-03 [38]	
	Copen Text Spreadsheet Spreadsheet setup	+	1052	SiO2(SLAGA)	FToxid	FToxid-SLAGA		6.8588E-02	6.8588E-02 [38]	0.8134 [1]	
	C Save Text Spreadsheet		1053	NaAlO2(SLAGA) CaO(SLAGA)	FToxid	FToxid-SLAGA		8.5125E-06	1.8802E-08 [1] 3.7994E-07 [1]	8.5125E-06 [38]	1
	Swap rows & columns		1055	FeO(SLAGA)	FToxid	FToxid-SLAGA		0.2781	0.1157 [1]	0.2781 [38]	
Cancel	ОК	+	1050	MgO(SLAGA)	FToxid	FT oxid-SLAGA		4.4240E 05 8.0697E-02	9.2915E-03 [1]	4.4240E 05 [30] 8.0697E-02 [38]	
			1058		Floxid	FT oxid-SLAGA		3.2034E-05	1.3708E-05 [1]	3.2034E-05 [38]	
preadsheet Setup	•		1059	MiD(SLAGA) MnO(SLAGA)	FToxid	FToxid-SLAGA FToxid-SLAGA		2.1544E-03	5.0847E-05 [1] 5.9400E-04 [1]	2.1544E-03 [38]	
System Properties			1061	CrO(SLAGA)	FToxid	FT oxid-SLAGA		1.4742E-02	9.8533E-03 [1]	1.4973E-02 [36]	
-,	Property columns 2		1062	Mn203(SLAGA)	FToxid	FToxid-SLAGA		3.3823E-04 3.7091E-10	1.1765E-11 [1]	3.7091E-10 [38]	-
Column: - 1 - Variable: Alpha	-2- T(C)	+'d	enotes al	I the Species Propert	ies as defin	ed in the Spreads	heet Se	etup.		_	
				Select	All		Clear		OK		
- Species Properties Columns per species 1	C order species order props.	Column	s: 4								
Column:	Select Species: 2	Cano Defa	el ult								



**Ferrous Processing 35** 

**McGill CRCT** 

-										
Fi	le Edit Swar	p rows and colum	ns							
Γ	Alpha	T(C)	Wt%-SiO2(SLAGA#1)	Wt%-MgO(SLAGA#1)	Wt%-SiO2(SLAGA#2)	Wt%-MgO(SLAGA#2)				
	1.2120000E+01	1.6000000E+03	5.9104840E+01	1.4772695E+01	5.9104840E+01	1.4772695E+01				
	1.2620000E+01	1.600000E+03	5.8497349E+01	1.5382513E+01	5.8497349E+01	1.5382513E+01				
	1.3120000E+01	1.600000E+03	5.7889996E+01	1.5992402E+01	5.7889996E+01	1.5992402E+01				
	1.3620000E+01	1.600000E+03	5.7282768E+01	1.6602366E+01	5.7282768E+01	1.6602366E+01				
	1.4120000E+01	1.600000E+03	5.6675654E+01	1.7212408E+01	5.6675654E+01	1.7212408E+01				
	1.4620000E+01	1.600000E+03	5.6068642E+01	1.7822534E+01	5.6068642E+01	1.7822534E+01				
	1.5120000E+01	1.600000E+03	5.5461721E+01	1.8432746E+01	5.5461721E+01	1.8432746E+01				
	1.5620000E+01	1.600000E+03	5.4854884E+01	1.9043049E+01	5.4854884E+01	1.9043049E+01				
	1.6120000E+01	1.600000E+03	5.4248124E+01	1.9653448E+01	5.4248124E+01	1.9653448E+01				
	1.6620000E+01	1.600000E+03	5.3641436E+01	2.0263948E+01	5.3641436E+01	2.0263948E+01				
	1.7120000E+01	1.600000E+03	5.3034815E+01	2.0874555E+01	5.3034815E+01	2.0874555E+01				
	1.7620000E+01	1.600000E+03	5.2428259E+01	2.1485276E+01	5.2428259E+01	2.1485276E+01				
	1.8120000E+01	1.600000E+03	5.1821769E+01	2.2096119E+01	5.1821769E+01	2.2096119E+01				
	1.8620000E+01	1.600000E+03	5.1215345E+01	2.2707092E+01	5.1215345E+01	2.2707092E+01				
	1.9120000E+01	1.600000E+03	5.0608990E+01	2.3318205E+01	5.0608990E+01	2.3318205E+01				
	1.9620000E+01	1.600000E+03	5.0002708E+01	2.3929470E+01	5.0002708E+01	2.3929470E+01				
	2.0120000E+01	1.600000E+03	4.9396507E+01	2.4540898E+01	4.9396507E+01	2.4540898E+01				
	2.0620000E+01	1.600000E+03	4.8790393E+01	2.5152504E+01	4.8790393E+01	2.5152504E+01				
	2.1120000E+01	1.600000E+03	4.8184375E+01	2.5764304E+01	4.8184375E+01	2.5764304E+01				
	2.1620000E+01	1.600000E+03	4.7578465E+01	2.6376315E+01	4.7578465E+01	2.6376315E+01				
	2.2120000E+01	1.600000E+03	4.6972673E+01	2.6988559E+01	4.6972673E+01	2.6988559E+01				
	2.2620000E+01	1.600000E+03	4.6367012E+01	2.7601056E+01	4.6367012E+01	2.7601056E+01				
	2.3120000E+01	1.600000E+03	4.5761495E+01	2.8213831E+01	4.5761495E+01	2.8213831E+01				
	2.3620000E+01	1.600000E+03	4.5156135E+01	2.8826909E+01	4.5156135E+01	2.8826909E+01				
	2.4120000E+01	1.6000000E+03	4.4550942E+01	2.9440317E+01	4.4550942E+01	2.9440317E+01				

Copy and paste in Excel file and then, you can calculate the ratio of SiO<sub>2</sub>/MgO in Slag Impossible to draw as a function of SiO<sub>2</sub>/MgO in FactSage



Equilib Results

Ferrous Processing 36

Save or Print  Plot	T(C) P(atm) Energy(J) Mass(g) Vol(litr	e) <u>I</u>	1 🖳 🖻 😿	Create 37 stream files for Slag
Equilib Results file	9.62 A=20.12 A=20.62 A=21.12 A=21.0	52 A=22.12 A=22.62 A=2	3.12 A=23.62	nhases
Stream File	Recycle all streams	A=16.12 A=16.62 A=17.7	12   A=17.62   '	phacee
Format 🕨	Save stream file	Save gas phase	6.3 🔺	
Fact-XMI	Stream file properties	Save pure liquids		
, act Ame	Summer of streams	Save aqueous		
Fact-Optimal	Summary of streams	Save pure solids		
East Eurotian Builder	Directory (C:\FactSage\)	Save solutions		lutions
Fact-Function-Builder	p =	5472 301410113	ALL SU	
Refresh	1,s1-Floxid,#1)		F5stel-	
9.2135E-03 mol gas ide	Pal		FSstel	-FCC1 FCC_A1
(0.26153 gram, 9.2135E-0	03 mol, 1.4162 litre, 1.8467E-04 g	ram/cm3)	<b>F</b> Sstel-	-BCC1 BCC A2
(1600 C, 1 atm,	a=1.0000)			
( 0.97654	co	FactPS	Floxic	I-SLAGA#1 ASlag-liq
+ 2.3284E-02	C02	FactPS	FToxic	I-SLAGA#2 ASlag-lig
+ 7.4306E-05	Fe	FactPS		
+ 6.5345E-05	SiO	FactPS	Floxic	I-SPINA#1 ASpinel
+ 3.1435E-05	Na	FactPS	FToxic	I-SPINA#2 ASpinel
+ 2.6810E-06	Ni	FactPS		
+ 1.3820E-06	Mg	FactPS	FToxic	I-MeO_A#1 AMonoxide
+ 8.1622E-07	Mn	FactPS	FToxic	I-MeO A#2 AMonoxide
+ 2.1625E-07	Cr	FactPS		
+ 9.9725E-08	FeO	FactPS	FToxic	I-cPyrA AClinopyroxene
+ 8.7642E-08	Co	FactPS	FToxic	l-oPyr Orthonyrovene
+ 5.7545E-08	5102	FactPS	TTOAL	-or yr orthopyroxene
+ 2.0547E-08	Cro	FactPS	FToxic	I-pPyrA AProtopyroxene
+ 1 6028E-09	Gr02	FactPS	FToxic	I-OlivA AOlivine
			Floxic	1-MulF Mullite



Ferrous Processing 37

FToxid-CORU#2 M2O3(Corundum)

🐯 McGill CRCT

Montreal

Re Re	actants	- Fauilib						3	FSstel-LIQU LIQUID stream
Eile .		Table Unite Date	- Saarah Hala					4	FToxide Slag stream
		dd a new Desetent	a search <u>H</u> eip	Child	<b>D</b>	bl(litre)		5	Slag with A=12.12 stream
	A	dd a new Keactant		Ctri+i	ĸ	Di(iide)		6	Slag with A=12.62 stream
	In	isert new reactant b	etore					7	Slag with A=13.12 stream
	D	elete reactant						8	Slag with A=13.62 stream
Г	D	elete all blank react	ants					9	Slag with A=14.12 stream
	M	lixtures and Streams	S		•	Import a mixture	•	1	0 Slag with A=14.62 stream
	Re	e-order the reactant	ts		•	Import a stream (or single-lin	ne mixture) 🔹 🕨	1	1 Slag with A=15.12 stream
	Ex	port list of reactant	ts		•	Edit a mixture or stream	•	1	2 Slag with A=16.12 stream
	In	nport list of reactan	ts		•	Directory (C:\FactSage\)		1	3 Slag with A=16.62 stream
	c	lear			-1			1	4 Slag with A=17.12 stream
	Ex	rample						1	5 Slag with A=18.12 stream
		ampic						1	6 Slag with A=19.12 stream
								1	7 Slag with A=20.12 stream
								1	8 Slag with A=21.12 stream
								1	9 Slag with A=22.12 stream
								2	0 Slag with A=23.12 stream
								2	1 Slag with A=24.12 stream
								2	2 Slag with A=25.12 stream
						🔽 Initial Co	nditions	2	3 Slag with A=26.12 stream
								2	4 Slag with A=27.12 stream
				Next >>				2	5 Slag with A=28.12 stream
5			Molet					2	6 Slag with A=29.12 stream
FactS	age 6.3	Compound: 3	3/19 databases	Solution: 2719 datab	ases			2	7 Slag with A=30.12 stream
Select each stream and calculate liquidus temp									8 Slag with A=30.3 stream
		001001		na (Procini	4-14	o Torgot'	···· P· ·	S	ilag FToxid-SLAGA#1 stream
		S	Steel FSstel-LIQU stream						



**Ferrous Processing 38** 



Menu - Equilib: 37 calculations								
File       Units       Parameters       Help         T(C)       P(atm)       Energy(J)       Mass(g)       Vol(litre)         Reactants       (1)       Image: Comparison of the second seco								
Products         Compound species         * + gas • ideal • real 34         aqueous 0         pure liquids 0         * + pure sol         Click mouse-right-b         suppress duplicates apply         * - custom selection         species: 148         Precipitate T arget         FT oxid-SLAGA         Estimate T(C): 1000         Mass(g): 0	Solution species	Custom Solutions 0 fixed activities 0 ideal solutions 0 activity coefficients Details Pseudonyms apply List include molar volumes <u>Total Species (max 1500)</u> 582 <u>Total Solutions (max 40)</u> 15 Default						
Final Conditions <a>         10       steps         Table         FactSage 6.3       C:\FactSage</a>	T(C) P(atm) Delta H(J) 1 1 1 1 1 2 2 2 2 2 2 2 2 2 2 2 2 2	quilibrium       normal						



Ferrous Processing 39

**McGill CRCT** 

Q	Results	- Equilib 1468.09 C			1000	
0	utput	<u>E</u> dit <u>S</u> how Pages				
[	0	Em ber f	T(C) P(atm) E	inergy(J) Mass(g) Vol(litre)		111 🞐 🕒 😿
		+ 29.353 w + 0.27335 w + 1.45748-02 w	t.% Fe1Cr204 t.% Cr1Cr204		FToxid FToxid	*
		+ 9.0725E-03 w + 9.0725E-02 w + 2.5892E-03 w	t.% Cr1Al204 t.% Cr1Al204 t.% Co1Al204		FToxid FToxid	
		+ 4.1180E-05 w + 8.9999E-11 w + 3.4195E-07 w	t.% Co1Fe2O4 t.% Co1Co2O4 t.% Fe1Co2O4		FToxid FToxid FToxid	
		+ 3.1984E-03 w + 5.0886E-05 w	t.% Ni1Al2O4 t.% Ni1Fe2O4		FToxid FToxid	
		+ 5.3608E-07 w + 7.7316E-03 w + 9.5535E-03 w	t.% Mg1Co2O4 t.% Co1Cr2O4 t.% Ni1Cr2O4		FToxid FToxid FToxid	
		+ 1.1121E-10 w + 3.1877E-09 w	t.% Ni1Co2O4 t.% Cr1Co2O4		FToxid FToxid)	
	+ 0	gram SiO2_ (1468.09 C, 1	cristobalite(h) atm, S6, a=1.0000)		FToxid	
	+ 0	gram SiO2_ (1468.09 C, 1	tridymite(h) atm, S4, a=0.99999)	)	FToxid	
	+ 0	gram SiO2_ (1468.09 C, 1	quartz(h) atm, S2, a=0.92034)	)	FToxid	
	+ 0	gram MgSiO (1468.09 C, 1	3_proto-enstatite atm, S3, a=0.54841)	)	FToxid	
	+ 0	gram MgSiO (1468.09 C, 1	3_ortho-enstatite atm, S2, a=0.54085)	)	FToxid	-

Primary crystallization phase is SiO<sub>2</sub> (cristobalite)

Using Macro function, this kind of calculation can be carried out automatically.

Repeat to calculate the liquidus temp of each slag using 'Precipitate Target'



Ferrous Processing 40

McGill CRCT

# The effect of $SiO_2/MgO$ and FeO and $AI_2O_3$ in Slag on the liquidus temperature of the Slag Phase Diagram / Equilib



Ferrous Processing 41

🐯 McGill CRCT

### Actually, SiO<sub>2</sub>/MgO of Laterite is almost same as that of the produced Slag The main system of Slag is virtually SiO<sub>2</sub>-MgO-Al<sub>2</sub>O<sub>3</sub>-FeO

Q (	Compon	ents - P	hase Diagram		-			
File	Edit	Units	Data Search	Help				
Ľ	2	+		Т	(C) P(atm) Er	hergy(J) Mass(g) Vo	l(litre)	111 📑 🕒 📧
	1 - 5				Cor	nponents		
				Г	Al2O3 Fe0 Fe		Note: - on the phase diagram the units of mass will be g, but the chemical formulae of the components remain molar values.	•
				Fe-sa	aturati	on cond	lition	
							Eh -	pH diagram
						Next >>		
Fac	Sage 6.3	) Co	ompound: 2	/19 databases	Solution:	2/19 databases		



Ferrous Processing 42

🐯 McGill CRCT

Selection - Equilib - no results -		Soloct pure solid and liquid of						
File Edit Show Sort		Select pure solid and liquid of						
Selected: 41/68 SOLID Duplicates selected.		Fe for Fe-saturation condition						
- no results -		i c ioi i c-saturation condition						
	Maximum 🔺							
18 SiO2(s) FSstel quartz(l) V		: comments						
19         SiO2(s2)         FSstel         quartz(h)         V           20         SiO2(s3)         ESstel         tridumite(l)         V		Variables Help						
21 SiD2(s4) FSstel tridymite(h) V								
22 SiO2(s5) FSstel cristobalite(I) V		T(C) P(atm) Energy(J) Mass(g) Vol(litre) 🛛 👖 🏢 🦳 🐺						
+ 24 Fe(s) F5stel cristobalite(h) V								
+ 25 Fe(s2) FSstel fcc_a1								
26 Fe2O3(s) FSstel hematite V								
27 Fe3U4(s) F5stel magnetite V 28 Fe3U4(s2) F5stel magnetite V		(gram) SiO2 + FeO + MgO + Al2O3 + Fe						
29 Al5Fe2(s) FSstel al5fe2 o								
30 Al61Fe31(s) FSstel al2fe o								
Show Selected     Select All     Select/Clear     Clear       Image: Show Selected     Image: Selected     Image: Selected     Image: Selected       Image: Selected: 1/10     LIQUID     Duplicates     selected       Image: Selected: 1/10     LIQUID     Selected: 1/10     Mage: Selected       Image: Selected: 1/10     Selected: 1/10     Selected: 1/10     Selected: 1/10       Image: Selected: 1/10     Selected: 1/10     Selected: 1/10     Selected: 1/10       Image: Selected: 1/10     Selected: 1/10     Selected: 1/10     Selected: 1/10       Image: Selected: 1/10     Selected: 1/10     Selected: 1/10	ок queous ure liquids ure solids	Solution species Solution spe						
+ 8 Fe(liq) FSstel liquid		solutions: 12 Default						
10 Mg0(liq) FToxid liquid								
11 Al2O3(liq) FToxid liquid		Phase Diagram						
12 SiO2(liq) FToxid liquid		Fe0/(Si02+Fe0 Al203/ Fe/(Si02+Fe0 A						
Intervision         Nacion         Intervision         Intervision <t< td=""></t<>								
		sNo4-Si02-Mg0-Al203-Si02-constant_1500C.DAT						



Ferrous Processing 43

**McGill CRCT** 

Variables: SiO2-MgO-Al2O3-FeO-Fe comp	osition #3. vs composition #1.		CALL IN MARK	
✓ariables     T and       Y          •         •         •	P erature Constant	/olume	ergy(J) Mass(g) Vol(litre)	M 🗩 🖶 🕱
B C C Y steps: 10 Next >>	1500 C V(litre) C log V		) + MgO + Al2O3 + Fe	- Custom Solutions
- Compositions (mass) #1. 1 SiO2 + 0 MgO + 0 Al 1 SiO2 + 1 MgO + 1 Al Composition #	$\frac{203 + 0}{100} Fe0 + 0 Fe}{203 + 1} Fe0 + 1 Fe} = \frac{X \cdot axi}{1 (ma)}$	ase ↓G/ N/ ×)	e     Full Name       A     ASlag-liq all oxides + S       A     ASpinel       A     AMonoxide       A     AMonoxide       A     AClinopyroxene       Orthopyroxene     Orthopyroxene       A     AProtopyroxene       A     AOlivine       Mullite     ▼	0 fixed activities 0 ideal solutions 0 activity coefficients Details Pseudonyms apply List include molar volumes <u>Total Species (max 1500)</u> 178 <u>Total Solutions (max 40)</u> 12
Canc		OK	species: 136 solutions: 12	Default
	- Variables		PI	hase Diagram
	T(C)         Si02/(Si02+Fe0)           1500         [0 1]	Fe0/(Si02+Fe0         Al20           01         0	03/ Fe/(Si02+Fe0 0 0.000001 B 4	Âc
	A = SiO2, B = MgO, C = FeO FactSage 6.3	sNo4-SiO2-Ma0-Al2O3-SiO2-	-constant 1500C.DAT	Calculate >>
	<b>2</b>	<b>-</b>		11



**Ferrous Processing 44** 

**McGill CRCT** 

Variables: SiO2-FeO-MgO-Al2O3-Fe composition #1. vs composition #1.	×
Variables YCompositionsImage: Composition for the second seco	Ternary phase diagram of FeO-MgO-SiO <sub>2</sub> at constant Al <sub>2</sub> O <sub>3</sub> with Fe-saturation
-Compositions (mass) 1 SiD2 + O FeO + O MgO + O Al2O3 + O Fe $\sim$	Variables: SiO2-MgO-Al2O3-FeO-Fe composition #3. vs composition #1.
#1. 1 SiO2 + 1 FeO + 1 MgO + 0 Al2O3 + 0 Fe Composition # #1 * max = 5 Cancel	Variables       Compositions 4         Y          • compositions 4         A       Iog10(a) ▼ 0         B       C         Y steps: 10       Next >>
	- Compositions (mass)
	#4.       U       SiO2 +       U       MgO +       U       Al2O3 +       U       FeO +       1       Fe       I constant       ✓         1       SiO2 +       1       MgO +       1       Al2O3 +       1       FeO +       1       Fe       =
Add small	Composition # #4 _ max = 4
	Cancel



Ferrous Processing 45

The second secon





Ferrous Processing 46

McGill CRCT

Montreal

Variables:SiO2-FeO-MgO-Al2O3-FeT(C) vs comVariables YcompositionsTand PY $\bigcirc$ Ccompositions $\blacksquare$ TemperatureA B $\bigcirc$ C $\bigcirc$ T(C) $\bigcirc$ T(C) $\bigcirc$ T(T)Ysteps: $\boxed{11}$ Next >>	Y-axis        Y-axis        Max:     2000       Min:     1000       C     log P       C     log V	With change 0 to 8 wt% of Al <sub>2</sub> O <sub>3</sub> at constant SiO <sub>2</sub> /MgO=1 under Fe-saturation
Compositions (mass)         #1       SiO2 + 0       FeO + 1       MgO +         1       SiO2 + 1       FeO + 1       MgO +         Composition #       #1       max = 4	0 AI203 + 0 Fe = constant 1 AI203 + 1 Fe 0	ature     Pressure or Volume       Y-axis     P(atm) constant       Max:     2000       Min:     1000       V(litre)     1       C     log V
Cancel	OK #3. 1 SiO2 + 1 FeO + 1 M Composition # #3 1 max =	+ 100 Al203 + 0 Fe constant g0 + 1 Al203 + 1 Fe 5 4
<b>Fact</b> Sage <sup>™</sup>	Ferrous Processing 47	Wontrea





Ferrous Processing 48

WCGill CRCT Montreal 2013

# Show the liquidus temperature of the alloy as a function of Fe-Ni grades

Precipitate target / Phase diagram



Ferrous Processing 49

🐯 McGill CRCT



### The alloy mainly contains Fe and Ni with small amounts of Co or Cr Virtually, it is a binary Fe-Ni system

Q I	Reactant	ts - Equ	ilib						
<u>F</u> ile	<u>E</u> dit	<u>T</u> able	<u>U</u> nits	<u>D</u> ata Search	<u>H</u> elp				
	2	+			T(C) P(atm	) Energy(J) Mass(g) V	/ol(litre)		ll 📑 🕒 📧
	1 - 2								1
	_	Ma	nss(g)		Species	Phase	T(C)	P(total)**	Stream# Data
	<1	00-A>		Fe					1
	* <a< td=""><td>&gt;</td><td></td><td>Ni</td><td></td><td></td><td><u> </u></td><td></td><td>1</td></a<>	>		Ni			<u> </u>		1
									Initial Conditions
ي ا									
						Next >>			
Fac	Sage 6.3	3 C	ompound	: 3/19 datab	ases Solutio	on: 2/19 databases			11



Ferrous Processing 50

🐯 McGill CRCT

Iontreal

存 Menu - Equilib: NO5-Liquidus c	of Fe-Ni	
File Units Parameters Help	T(C) P(stm) Energy(I) Mass(a) )(allitra)	
Beactants (2)	r(c) r(aunij Energy(d) Massigji Voljuce)	
	(gram) <100-A> Fe + <a> Ni</a>	
Products		
Compound species         + gas • ideal C real       2         aqueous       0         pure liquids       0         + pure solids       6	Solution species       *     Base-Phase       P     FSstel-LIQU       +     FSstel-FCC1       +     FSstel-FCC1       +     FSstel-BCC1       BCC_A2	Custom Solutions 0 fixed activities 0 ideal solutions 0 activity coefficients Details
suppress duplicates apply species: 8		Pseudonyms apply List
Precipitate Target FSstel-LIQU Estimate T(C): 1000 Mass(g): 0	Legend       Image: Constraint of the selected         P - precipitate target       + - selected       Show O all ● selected         + - selected       2       species: 6 solutions: 3       Select	<u>Total Species (max 1500)</u> 14 <u>Total Solutions (max 40)</u> 3 Default
Final Conditions <a>           0 50 1           10         steps</a>	T(C) P(atm)	quilibrium       normal     C normal + transitions       transitions only       open       Calculate >>
FactSage 6.3 C:\FactS	age\EquiNO5-Liquidus_of_Fe-Ni.DAT	



Ferrous Processing 51

**McGill CRCT** 

Results - Equilib 1537.81 C, A=0 (page 1/51)										
Output Edit Show Pages										
Save or Print   T(C) P(atm) Energy(J) Mass	(g) Vol(litre)	111 🖳	🕒 😿							
Plot  Plot Results										
Equilib Results file         Repeat Plot - T(C) vs Alpha           Stream File         1000.72 C, A=14         1498.08 C, A=1           Format         512.78 C, A=8         1510.81 C, A=9         15           0.86 C, A=2         1527.08 C, A=3         1522	52 C, A= 52 C, A= 53 C, A= 54 C, A= 54 C, A= 55 C,	22   1482.54 C, A=23   essor: C:\FactSage\Equi0.	res	×						
Fact-XML	_	<100-A>Fe+ <a></a>	Ni	<u> </u>						
i =	Axes	Variables	Minimum	Maximum						
Fact-Optimal		activity	0	1.						
a1		mole	0	1.7907						
Fact-Function-Builder ▶ n, a=3.6413E-05)		mole fract.	0	1.						
Fe		gram	0	100.						
Kefresh		weight %	0	100.						
(100 gram 1 7907 mol)		Alpha	0	50.						
(1537.81 C, 1 atm, a=1.0000)		T(C)	1445.9	1537.8						
(100.00 wt.% Fe		P(atm)	1.	1.						
		Cp(J)	75.575	82.369						
System component Mole fraction Mass	fi	G(J)	-1.9775E+05	-1.9378E+05						
Fe 1.0000 1.	00(	Vol(litre)	0	0						
+ 0 gram BCC 33		H(J)	1.0825E+05	1.2976E+05						
(1537 81 C 1 atm a=1 0000)		V(litre)	0	0						
(100.00 wt.% Fe1Va3		S(J)	176.13	180.43						
		- page -	1.	51.						
+ 0 gram FCC_A1 (1537.81 C. 1 atm. a=0.99446)	Axes	Species	- Graph	alau						
( 100.00 wt.% FelVa1 + 0 gram Fe_bcc_a2 (1537.81 C, 1 atm, S1, a=1.0000)	0 selected Axes	O selected       Select       Repeat	Labels size: 9 no: 4 chemical integer # O none	color full screen reactants O Viewer file name © Figure						
	FactSage 6.3	C:\FactSage\Equi0.res		5Feb13 51 sets						



Ferrous Processing 52

**McGill CRCT** 

	Show	Select												
۰T	#	Species	Mole (min)	Mole (max)	Fraction (min)	Fraction (max)	Acti	vity (min)	Activity (max)					
6	ias	<u>Phase</u>												
	1	Fe(g)	0	0	0.751736	1.	4.547	71E-06	3.6413E-05					
	2	Ni(a)	0	0	0	0.248264	0		1.5017E-06					
F	Sstel-	<u>LIQU</u>												
1	3	Fe(LIQU)	0.895335	1.7907	0.512434	1.	0.473	824	1.					
Ŀ	4	Ni(LIQU)	0	0.851885	0	0.487566	0		0.398546					
Ľ	5stel-	<u>FLLI</u>						•						
!	5	Fe1Va1(FCC1)	0	0	0.518534	1.	-A	Results Pro	cessor: C·\FactSa		ui0 res			Σ
	6	Ni1Va1(FCC1)	0	0	0	0.481466	<b>_</b>	nesones i re	cesson en actou	90,00	aioires			
ŀ	<u>-Sstel-</u>	BCC1			0.500000		<u> </u>	e <u>H</u> elp						
	/ D	FerVa3(BCCT)	0	0	0.598803	1.			2100-65	Fe +	ZAN Ni		_	
	5 )	NITVA3(BCCT)	U	U	U	0.401197	-		R100A/	101	V-2 10			
	rure	<u>50lids</u> Eo(a)	0	0	0	0		Axes	Variables		A I	linimum		Maximum
	5 10	Fe(s) Fe(s2)	0	0	0	0			activ	ity		0		1.
	11	re(sz) Ni(e)	0	0	0	0				la		0		1 7907
	12	Fe(s)	0	0	0	0			Axes: T(C)	vs A	lpha			
	13	Fe(s2)	0 0	n	ñ	ů.				, .				
		()	-		-	-			Y-variable X	-varia	able Swap Ax	es		
				Mas	-Order									
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				[ [page] ] O d	iram C mass	(max)				T(C)		4	Alpha	
	Class	. 1			C fractio	on (max)	-							69
	Liea			51 pages	<ul> <li>activi</li> </ul>	ty (max) 56			maximum	154	0	maximum	50	BE+05
lic	k on the	+' column to add o	r remove species.						minimum	144	5	minimum	Ο	
_											<u> </u>			6E+05
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**Ferrous Processing 53** 

**McGill CRCT** 





Ferrous Processing 54

**McGill CRCT** 

Montreal

# The effect of Fe-Ni grades on the concentration of Co and Cr in the liquid alloy Equilib Calculation



Ferrous Processing 55

**McGill CRCT** 

🕞 Reactants - E	quilib										
File Edit Tab	le Units D	)ata Search Help									
🗅 🚔 +		T(C	) P(atm) Energy(J) Mass(g) Vol(	litre)		<b> </b>	🦻 🖪				
	1.10 11.14										
1.10   11.	14						1				
	Mass(n)	Snecie	s Phase	T(C)	P(total)**	Stream#	Data				
8,1	(9)	FeO	solid-FactPS wustite	▼ 500	1	1	FactPS				
+ 20,9		Fe203	solid-1-FToxid hematit	▼ 500	1	1	FToxid				
+ 43.8		Si02	solid-1-FToxid quartz(I	▼ 500	1	1	FToxid				
+ 6.4		AI203	solid-4-FToxid corund	▼ 500	1	1	FToxid				
+ 16.8		MgO	solid-FT oxid periclase	▼ 500	1	1	FToxid				
+ 2.3		NiO	solid-FT oxid	▼ 500	1	1	FToxid				
+ <4.8A>		AI203	solid-4-FToxid corund	▼ 100	1	2	FToxid				
+ <14A>		Si02	solid-1-FToxid quartz(l	▼ 100	1	2	FToxid				
+ <81.2A>		C	solid-1-FactPS graphit	▼ 100	1	2	FactPS				
+ 0.1		CaO	solid-FT oxid lime	▼ 500	1	1	FToxid				
					•	Initial Condit	ions				
			Next >>								
FactSage 6.3	Compound:	3/19 databases	Solution: 2/19 databases								



Ferrous Processing 56

**McGill CRCT** 

Menu - Equilib: change of Ni w	ith adding Char										
File Units Parameters Help											
🗅 🚘 🔚 T(C) P(atm) Energy(J) Mass(g) Vol(litre) 👖 📑 📑 🖏											
Reactants         (14)           (gram)         8.1         FeO         +         20.9           (500C,s-FactPS,#1)         (500C,s	Fe2O3 + 43.8 SiO2  -FToxid,#1) (500C,s1-FToxi	2 + 6.4 Al2O3 d,#1) (500C,s4-FToxid,#1	+ 16.8 MgO + ) (500C,s-FToxid,#1) (50								
Products Compound species	┌─ Solution species		Custom Solutions								
* ∓ gas ⊙ideal ⊖ real 51	· Base-Phase	Full Name 🔺	0 fixed activities								
aqueous 0	+ FSstel-LIQU		0 ideal solutions								
pure liquids 0	+ FSstel-FCC1	FCC_A1	U activity coefficients								
★ + pure solids 116	+ FSstel-BCC1	BCC_A2	Details								
suppress duplicates apply	I FToxid-SLAGA	ASlag-liq all oxides + S	Desudences								
* - custom selection	I FT oxid-SPINA	ASpinel	- Fseudonyms								
species: 167	I FToxid-MeO_A	AMonoxide	apply List								
	+ FToxid-cPyrA	AClinopyroxene	🗖 inaluda malar yakumaa								
	+ FToxid-oPyr	Orthopyroxene									
- Target	Legend I - immiscible 4	Show C all 💿 selected	Total Species (max 1500) 584 Total Solutions (max 40) 16								
Estimate ALPHA: 1 Mass(g): 0	+-selected 8	species: 417 solutions: 16 Select	Default								
- Final Conditions			auilibrium								
(A) <b> T(C) P(atm) ▼ Delta H(I) ▼ Onormal C normal + transition</b>											
0.0.1.0.005	1600 1		transitions only								
10 steps Table	11000	21 calculations	open Calculate >>								
FactSage 6.3 C:\\E(	uiNo6-Fe-Ni_effect_on_Co_and_C	Cr_composition.DAT									

With change of Char, Fe-Ni grade will be changed. The effect of Fe-Ni grades on the solubility of Co and Cr can be calculated with change of Char.

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2013



Ferrous Processing 57



### **Gact**Sage<sup>™</sup>

#### Ferrous Processing 58

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<b>)</b> S	Species Selection - EQUILIB Results: weight % vs Alpha									
File	Show	Select								
+	#	Species	Gram (min)	Gram (max)	₩t.%	(min)	₩t.% (max)	Activity (min)	Activity (max)	▲
	53	C(LIQU)	0	0.172327	0		0.697922	0	7.3983E-04	
+	54	Co(LIQU)	0	7.8630E-02	0.21442	1	1.4707	1.2119E-06	1.3862E-02	
+	55	Cr(LIQU)	0	0.384669	3.4297E-05		1.5579	7.7175E-11	1.3032E-02	
	56	AI(LIQU)	0	5.1829E-05	2.3078E	Pocult	×			
	57	Mn(LIQU)	0	3.8302E-02	4.7114E	Result	S Processor: C:\raci	sage (Equivires	100 C 100	
+	58	Ni(LIQU)	0	1.8073	7.3194	File He	lp			
	59	SI(LIQU)	0	1.4944	1.37518		81 F	eO + 209Fe2O3+ 4	13 8 SiO2 + 6 4 Al2O3	+
	60	Mg(LIQU)	0	9.3987E-07	6.51858					
	61		0	9.6386E-03	4.27198	Axes	Variabl	es	Minimum	Maximum
	62	Alo(LIQU)	0	1.6660E-06	3.13116		a	stivity	0	104.58
	63	AI2O(LIQU)	0	1.4529E-09	2.60096			mole	0	2.5887
	64		0	3.5027E-04	3 47328	I	mole	fract.		0.999983
	65	Cr20(LIQU)	0	2.0450E-05	1 84176			gram	U	99.429
	66	MpO(LIQU)	0	1.57965-06	3 73685		Wei	gnt %	0	99.998
	67	SID(LIDLI)	0	3 5940E-04	7 59828	I	/	T(C) 1600		100
	07 CO	MaQ(LIQU)	0	2 2204E 05	C 00500			(ctm)	1000.	1600.
	CQ		0	1.01025.12	2 50070		Delta	(aun) Co(l)	19.62	82.696
	70		0	0.00045.10	2.03076		Delta		-3 8924F+05	-2 7358E±05
	70		U	8.9324E-10	2.28906		Vo	l(litre)	0.0024E+00	-2.73302403
							Delta	a H(J)	1.7769E+05	3.1154E+05
					s –		Delta	Vílitr	3.702	101.96
		C mole				Delta S(J)		a S(J)	152.43	277.68
				🗆 [page] 🛛 💽 gr	am		- P	age -	1.	21.
	Clea	r		21 pages		Axes	Specie	sGra	aph	ieplau
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	lick on the	e + column to add or	remove species.					si	ze: 9 no: 4	reactants O Viewer
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							Select species a	na phases to be plo	tted.	
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Ferrous Processing 59







Ferrous Processing 60

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Blow-up Scale of the solubility of Co and Cr with change of Char and Fe-Ni grade.

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