Case 3: Ilmenite (FeTiO₃) Smelting



Ferrous Processing 1

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Ilmenite is a mixture of FeO and TiO_2 . Canada currently has one of the largest ilmenite deposits. This ilmenite is processed by Rio Tinto Iron and Titanium (QIT) in Sorel, Quebec.

The main reactions occurring during ilmenite smelting is the reduction of FeO from slag to metal:

 $FeO(I)+C(s) \rightarrow Fe(I)+CO(g)$

and the partial reduction of TiO_2 in the slag: TiO₂(I)+0.5C(s) \rightarrow TiO_{1.5}(I)+0.5CO(g)

The ideal product would be a pure TiO2 slag and pure Fe metal.



In the following slides, we will study this reaction and analyze the smelting products.



Ferrous Processing 2

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1. We will assume that the ore is composed of pure ilmenite

F Reactants - Equilib	
<u>File E</u> dit <u>T</u> able <u>U</u> nits <u>D</u> ata Search <u>H</u> elp	🕝 Data Search 🛛 🔀
□ 🖻 🕂 💷 T(C) P(atm)	-Databases - 3/19 compound databases, 2/19 solution databases
1-2	Gact GactSage" SGTE compounds only Miscellaneous
	FactPS FScopp BINS Solutions only SGTE# SGTE*
Mass(g) Species	Elsalt FSlite SGTE Clear All
100 FeTIO3	Finall FSnobl Select All
	FIUxCN FSupsi Stinucl
	Add/Remove Data
	Filite FTdemo TDnucl RefreshDatabases
2. We will make the	- Information -
amount of carbon	3. Select FTmisc for the liquid iron
variable	solution and FToxid for the slag
	O-Martine -
	Include I
	Default aqueous species Minimum solution components: O 1 O 2 cpts
EastSage 6.2 Compound: 2/19 databases Colution	Cancel Summary OK
racioagelo.o Compound. o/15 databases Solutio	



Ferrous Processing 3

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1675 as the final temperature.



Ferrous Processing 4

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1. After calculation, it is found that solid pseudobrookite is precipitated.

2. It is necessary to select the right amount of carbon to avoid precipitation of pseudobrookite

3. This can be done using "Formation target"

🕞 Results	- Equilib 1675 C				
<u>O</u> utput <u>E</u> d	it <u>S</u> how Pages				
	I	T(C) P(atm) Energy((J) Mass(g) Vol(litre)		11 🖳 🗗 😿
	Fe2+	7 4246R-02	mos.		<u> </u>
	Fe3t	1.6055E-04			
	Ti3+	0.56792			
	Ti4+	0.35767			
	0	1.0000			
	System component	Mole fraction	Mass fraction		
	Fe	2.8166 E- 02	5.5605 E- 02		
	Ti	0.35038	0.59290		
	0	0.62146	0.35150		
		• •.			
+ 17.8	SU gram Pseudobro SEO gram 7 97478-02 m/	okite			
(17.	/1675 C 1 otm	9=1 0000\			
	(1.4500 wt.%)	TeTi205[2-]		FToxid	
	+ 49.907 wt.%	[i305[+]		FToxid	
	+ 1.5362 wt.% 1	FeTi205		FToxid	
	+ 47.107 wt.* 1	[i305[-]		FToxid)	
	Site fraction of su	ublattice constitue	ents:		
	Fe	2.8863 E- 02			
	TI3	0.97114			
	 TI4	0.51443			
	TI3	0.48557			
	System component	Mole fraction	Mass fraction		
	Fe	3.6078 E -03	7.2012 E -03		~
<u> </u>					



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Calculating the optimum amount of carbon addition: Pseudobrookite formation target



Ferrous Processing 6

The second secon

1. Right-click on	This example can be found in EquiCase3-1.dat
psoudobrookito	F Menu - Equilib: last system
pseudobiookite	Eile Units Parameters Help
selection	🗅 🚅 🖬 T(C) P(atm) Energy(J) Mass(g) Vol(litre) 👖 🖶 🕞 😿
	Reactants (2)
	(gram) 100, FeTiO3 + <1065, C
2. Select	
"Formation target	Products
nhaao"	Compound species Custom Solutions
phase	Solution FToxid-PSEU * Base-Phase Full Name O trixed activities
	- clear
	- all species FToxid-SPINA ASpinel
	- merge alloce solution from - FToxid-CURU M2U3(Corundum) apply List
	✓ + - single phase F FToxid-PSEU Pseudobrookite ✓
	I - possible 2-phase immiscibility Legend
	J - possible 3-phase immiscibility I - immiscible 1 Show C all C selected <u>I total Solutions (max 40)</u> 10
	- standard stable phase F - formation target species: 38 Select A
	! - dormant (metastable) phase Default Default
	→ ✓ F - formation target phase
	P - precipitate target phase
	S - Schell cooling target phase 100 r (atin) r roduct r(b) C transitions only
	C - composition target
	Help
	FactSage 6.3



Ferrous Processing 7

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1. Leaving <A> blank, a solution will be found for the value of <A>, where the activity of pseudobrookite will be 1, but its amount will be 0.

2. Note that the amount of carbon was changed to <10A> to allow carbon amount to change from 0 to 10g during the calculation.							
Reactants (2)	T(C) P(atm) Energy(J) Mass(g) Vol(litre)	11 📑 📑					
Products Compound species + gas ● ideal ○ real 17 aqueous 0 pure liquids 0 * + pure solids 41 ✓ suppress duplicates apply * - custom selection species: 58 Formation Target FToxid-PSEU Estimate ALPHA: 0.5 Mass(g): 0	Solution species * • Base-Phase Full Name + FTmisc-FeLQ Fe-liq I FToxid-SLAGA ASlag-liq all oxides + S + FToxid-SPINA ASpinel + FToxid-ORU M203(Corundum) + FToxid-TiO2 Rutile + FToxid-TiO2 Rutile + FToxid-PSEU Pseudobrookite F FToxid-PSEU Pseudobrookite Legend I Formation target I - iselected 7 Show @ all @ selected solutions: 10 Select	Custom Solutions 0 fixed activities 0 ideal solutions 0 activity coefficients Details Pseudonyms apply List 1 include molar volumes <u>Total Species (max 1500)</u> 96 <u>Total Solutions (max 40)</u> 10 Default					
Final Conditions <a> 10 steps Table FactSage 6.3	T(C) P(atm) ✓ Product H(J) ✓ 1675 1 1 1 1 calculation 1 1	quilibrium normal					

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1. Looking at the slag composition, it can be noted that the slag contains about 7% FeO

	4	F Results - Equilib 1675 C , A=	0.9741			
	9	Output Edit Show Pages				
			T(C) P(atm) Energy(J) Mass(g)	Vol(litre)	III 🖳 🦱 😿
	1					
		PHASE: ASlag-liq#1	gram	MASS FRACTION	ACTIVITY	~
		FeO	3.7983 E+ 00	→ 7.1382E-02	2.6445 E -02	_
		Fe203	9.1279 E- 03	1.7154E-04	3.1829 E- 08	
		Ti203	2.9063 E+ 01	5.4618E-01	2.2613 E- 01	
		TiO2	2.0341 E+ 01	3.8227E-01	3.3919 E- 01	
		TOTAL:	5.3211 E+ 01	1.0000E+00	1.0000E+00	
se.		PHASE: ASlag-liq#2	gram	MASS FRACTION	ACTIVITY	
,		FeO	0.0000 E+ 00	7.1382 E -02	2.6445E-02	
		Fe203	0.0000 E+ 00	1.7154E-04	3.1829 E- 08	
		Ti203	0.0000 E+ 00	5.4618E-01	2.2613 E- 01	
8%		Ti02	0.0000 E+ 00	3.8227 E- 01	3.3919 E- 01	
• / •		TOTAL:	0.0000E+00	1.0000E+00	1.0000E+00	
		PHASE: Fe-liq	gram	MASS FRACTION	ACTIVITY	
			3 38428+01	→ 9.9758E-01	9.8884E-01	
			7.62978-02	2.2490K-03	7.5501K-03	
			2.7909 E -03	8.2268K-US	3.69838-06	
		11	2.62398-03 2.75678.04	7.7345E-US	3.1673K-06	
		110 T+20	2.75678-04 5.49628-07	8.1261K-06 1 6025K-00	7.04328-06	
		1120 TOTAL-	3.4362B-07 3.2924B101	1.00238-00	1 00008400	
50		DHISE: Decudobrookite	3.3924BT01	MASS RDACTION	ACTIVITY	
hd		Fati20512-1	0 00008+00	1 4500F-02	2 67578-03	
IG I		Ti305(+)	0 00008+00	4 99078-01	2 50368-01	
on		FeTi205	0 00008+00	1.53628-02	1 84358-02	
		Ti305[-1	0.0000 E+ 00	4.7107E-01	2.3541 E- 01	
hon		TOTAL:	0.0000E+00	1.0000E+00	1.0000E+00	
		PHASE: Rutile	gram	MASS FRACTION	ACTIVITY	
		Ti203	0.0000 E+ 00	1.8825 E -01	3.7713E-01	
		Ti02	0.0000 E+ 00	8.1175E-01	4.3228E-01	
		TOTAL:	0.0000 E+ 00	1.0000 E+ 00	5.4369E-01	~
		· · ·				

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 It would be interesting to see how the slag and metal composition changes with carbor addition



Visualizing the change in metal and slag composition with carbon addition



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A series of calculations at different carbon addition is performed to see how carbon content affects the composition of metal and slag.

Elle Units Barameters Help Image: Sector Secto	Elle Units Prameters Elle Image: Section species T(C) P(atm) Energy(J) Mass(g) Vol(litre) Image: Section species Image: Section species Image: Section species Image: Section species Image: Section species Image: Section species Solution species Image: Section species Image: Section species Image: Section species Image: Section species Section species Section species Image: Section species Image: Section species Section species Image: Section species Image: Section species Image: Section species Image: Section species Section species Image: Section species Image: Section species Image: Section species Image: Section species Section species Section species Image: Section species Section species Section Section species Image: Section species Section Section species Section Sec	🖡 Menu - Equilib: last system		
Reactants (2) (gram) 100 FeTiO3 + <10A> C Products Solution species + gas (* ideal real 17) * Base-Phase Full Name * aqueous 0 pure liquids 0 ftoxid-SLAGA ASlag-liq all oxides + S 0 fixed activities * pure solids 41 * FToxid-SLAGA ASlag-liq all oxides + S 0 activity coefficients * suppress duplicates apply * FToxid-CORU M203(Corundum) * Pseudoprookite * * FToxid-TiO2 Rutile * Pseudoprookite * * include molar volumes Target * rowid-TiSp Titania_Spinel *	Reactants (2) (gram) 100 FeTiO3 + <10A> C Products Compound species Custom Solutions + gas • ideal real 17 Solution species Custom Solutions + pure solids 0 + FToxid-SLAGA ASlag-lig all oxides + S Custom Solutions • pure liquids 0 + FToxid-SLAGA ASlag-lig all oxides + S Custom Solutions • pure solids 41 • FToxid-SPINA ASpinel • Custom Solutions • suppress duplicates apply • FToxid-SPINA ASpinel • etails • Pseudonyms • custom selection • FToxid-TiC2 Rutile • rowid-PSEU Pseudobrook/ite • include molar volumes Target · none - · Egend · Show O all • selected · selected · selected · selected · mass(g) • more definitions • T(C) Product H(J) • · ormal · normal + transition (AA) • T(C) P(atm) · Product H(J) • · ormal · normal + transition	Eile Units Parameters Help	T(C) P(atm) Energy(J) Mass(g) Vol(litre)	11 💷 🖻
Products Compound species + gas (• ideal) real 17 aqueous 0 pure liquids 0 + pure solids 1 FToxid-SLAGA ASlag-liq all oxides + S 0 + FToxid-SLAGA * + Pure solids 1 * + FToxid-SPINA ASpinel * + FToxid-CORU M203(Corundum) * + FToxid-TiO2 Rutile * + FToxid-ILMEA Allmenite * + FToxid-TiSp Titania_Spinel * + FToxid-TiSp Titania_Spinel * + FToxid-TiSp Titania_Spinel * + selected 8 * Show 0 all (• selected * - selected 8 * selected * - selected 8 * selected	Products Compound species + gas • ideal • real 17 aqueous 0 pure liquids 0 + pure solids 1 + FToxid-SPINA ASpinel + FToxid-COBU M203(Corundum) + FToxid-TiO2 Rutile + FToxid-TiO2 Rutile + FToxid-TiSp Titania_Spinel - none - - Estimate ALPHA: 05 Mass(g): - + selected 8 - solutions: 10 Solutions: 10 Solutions: 10 Default - - conditions - - - normal + transitio - - normal + transitio - - normal + transitio - - ormal + transitio - - 01 0.01	Reactants (2)	(gram) 100 FeTiO3 + <10A> C	
+ gas (* lucar's real 17 - + Base-Fnase Full Name - aqueous 0 1 FToxid-SLAGA ASlag-liq all oxides + S 0	Image: sector of the sector	Products Compound species	Solution species	Custom Solutions
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Target + FToxid-PSEU Pseudobrookite include molar volumes Target + FToxid-TiSp Titania_Spinel Include molar volumes - none - - - Estimate ALPHA: 0.5 Mass(g): 0 - - Select Default - - - -	+ FT oxid-PSEU Pseudobrookite - none - - - - Titania_Spinel Include molar volumes - none - <	v suppress duplicates apply * - custom selection species: 58	+ FToxid-CORU M2O3(Corundum) + FToxid-TiO2 Rutile + FToxid-ILMEA Allmenite	Pseudonyms apply List
Estimate ALPHA: 0.5 Mass(g): 0 + - selected 8 species: 38 solutions: 10 Default Default	Estimate ALPHA: 0.5 + - selected 8 species: 38 Select Default Mass(g): 0 </td <td>- Target - none -</td> <td>+ FToxid-PSEU Pseudobrookite + FToxid-TiSp Titania_Spinel Legend ✓ I - immiscible 1</td> <td>include molar volumes <u>Total Species (max 1500)</u> <u>Total Solutions (max 40)</u></td>	- Target - none -	+ FToxid-PSEU Pseudobrookite + FToxid-TiSp Titania_Spinel Legend ✓ I - immiscible 1	include molar volumes <u>Total Species (max 1500)</u> <u>Total Solutions (max 40)</u>
	Final Conditions Equilibrium <a> T(C) P(atm) Product H(J) • normal • normal + transitions only 0 1 0.01 1675 1 • normal • normal • normal + transitions	Estimate ALPHA: 0.5 Mass(g): 0	+ - selected 8 species: 38 Select solutions: 10	Default
To steps Table 101 calculations Calculate >:		FactSage 6.3		

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1. For a graphical representation, we will plot the results

F Results - Eo	quilib A=0	(page 1/	/101)						×		
Output Edit Sh	how Pages										
Save or Print	► I		T(C) P(atm) E	nergy(J) Mass(g) Vol(litre)			- tit 💷 🗭 👿			
Plot	•	Plot Result	s		A-0.21 A-0.22						
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Stream File	· · · ⊺ <	Plot:	weight % vs Alph	a		<u>F</u> ile	Show S	jelect			
Format	► E	<u>F</u> ile <u>H</u> elp				+	#	Species	Mole (min)	Mole (max)	Fraction (min)
Fact-XML	•		100 FeTiO	3 + <10A> C			15	Fe(g)	0	1.7057E-04	7.9178E-06
							16	FeO(g)	0	2.2425E-07	6.8808E-08
Fact-Optimal	•	Axes	Variables		Minimum		17	Fe(CO)5(g)	0	3.4462E-25	0
Eact-Eunction-	Builder 🕨		activity		0		FTmisc	<u>FeLQ</u>			
			mole fract		0		18	Fe(FeLQ)	0	0.622743	0.80506
Refresh			dram		0		19	C(FeLQ)	0	6.5279E-03	0
	+ 2 6912	Y-axis	weight %		0		20	O(FeLQ)	0	6.7345E-04	2.8475E-04
	+ 4.0213	X-axis	Alpha		0		21	Ti(FeLQ)	0	5.6330E-05	7.2890E-10
l 1					1675.		22	TiO(FeLQ)	0	4.4356E-06	3.5772E-07
	2 5	elect	wt% as		1.		23	Ti2O(FeLQ)	0	4.9998E-09	7.6410E-19
+ 100.00	2.0	CICCI	W170 as		99.803		FT oxid	<u>SLAG</u>			
(100.00	the	e Y-ax	kis and		-1.2566E+06	+	24	FeO(SLAGA#1)	3.3863E-02	0.649684	0.103701
	Alpha as the X-axis			0	+	25	Fe2O3(SLAGA#1)	3.6612E-05	2.8092E-02	1.1212E-04	
				-6.0397E+05	+	26	Ti2O3(SLAGA#1)	2.8092E-02	0.201271	2.2258E-02	
l l				0	+	27	TiO2(SLAGA#1)	0.16313	0.602968	0.375718	
	+ 48.156		S(J)		268.1	1	FT oxid	<u>SLAG</u>			
			- page -		1.		28	FeO(SLAGA#2)	0	0	0.103701
	Site fra	- Akes	Species	Gra	aph		29	Fe2O3(SLAGA#2)	0	0	1.1212E-04
	Fe2+ Fe3+ Ti3+ Ti4+ O		t % 4 selecte		abels ize: 9 no: 4 chemical integer # none		3. Se C(Clea	elect all S omponent	lagA S	Source Mas (page) C g 101 pages	ss Order nole © integ gram © fracti © activ
	ŀ	-actSage Б.	3 U:\FactSage\Eq	ulU.res							



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2. The compositions remain constant after a certain point. This is when pseudobrookite precipitates.

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3. Because TiO₂ slag is the more important product of ilmenite smelting, we will select the amount of carbon to be 9.7g to keep wt%FeO at a minimum



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Visualizing the distribution of elements between phases: The "List" window



Ferrous Processing 16 🛛 🐯

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1. A good way of seeing the distribution of the elements between phases is by clicking on the "List" button...

	€ Li	ist - Eo	quilib T(C) = 1675, F	P(atm) =	1 (P	age 1/101)			(
	Eile	le <u>E</u> dit <u>H</u> elp						\mathbf{h}		
		È		Τ(0	C) P(atm) E	inergy(J) Mass(g) Vol(litre)			🕒 😿	
		Code		Data		Mole	Gram	Per Cent	Cumulate	T 🔺
	C.				Totals	0.0000	0.0000	0.0000 %		
	Ľ		TOTAL C			0.0000	0.0000			
			ELEMENT Fe			Mole Fe	Gram Fe	Per Cent	Cumulate	
			GAS PHASE							
					Totals	0.0000	0.0000	0.0000 %		
			FTmisc-FeLQ							
					Totals	0.0000	0.0000	0.0000 %		_
			FToxid-SLAGA						01.5.0	_
	-	97	FeU	Floxid		0.6030	33.67	91.48 %	91.5 %	-
	Fe	98	Fe2U3	Floxid	.	5.6184E-02	3.138	8.524 %	100. %	
			FT :101404		l otais	0.6592	36.81	100.0%		-
		F I OXID-SLAGA		T	0.0000	0.0000	0.00.00		_	
		_			l otais	4	4000/			
						4	100% (ot Fe is	in the s	iag
			3. It is now po	ssible	e to 占					_
		see that at <a>=0			0.0000	0.0000	0.0000 %		•	
		Show Format C mole						Order Code		
2and selecting	Г Г	liquid aque	0 viselected 9	6		C poun C data	d	C fraction C activity	of 101 pages	
alstribution	Ĺ	soluti	on 38 — All/Clear	j ⊽ pi	roperties	Post-Ca	ty	OK		

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1. And this is the distribution at <A>=0.49

D	🗅 🗃 T(C) P(atm) Energy(J) Mass(g) Vol(litre) 👖 📑 💽 😿						X			
	Code		Data		Mole	Gram	Per Cent	Cumulate	T	•
		ELEMENT Fe			Mole Fe	Gram Fe	Per Cent	Cumulate		
		GAS PHASE								
	15	Fe(g)	FactPS		8.4795E-05	4.7354E-03	1.2864E-02 %	1.286E-02 %		
	16	FeO(g)	FactPS		2.2389E-07	1.2503E-05	3.3967E-05 %	1.290E-02 %		
	17	Fe(CO)5(g)	FactPS		1.4702E-25	8.2104E-24	2.2305E-23 %	1.290E-02 %		
				Totals	8.5019E-05	4.7479E-03	1.2898E-02 %			
		FTmisc-FeLQ								
	91	Fe	FTmisc		0.2968	16.57	45.02 %	45.0 %	Т	
Ea				Totals	0.2968	16.57	45.02 %			
ге		FToxid-SLAGA								
	97	FeO	FToxid		0.3594	20.07	54.52 %	99.6 %	Т	
	98	Fe203	FToxid		2.9178E-03	0.1629	0.4427 %	100. %	Т	
				Totals	0.3623	20.23	54.96 %			
		FToxid-SLAGA								
				Totals	0.0000	0.0000	0.0000 %			
		FToxid-SPINA								
				Totals	0.0000	0.0000	0.0000 %			
		FToxid-MeO_A								-
FT oxid-Me0_A Show Species G mole gas 17 ✓ duplicate liquid 0 ✓ selected 96 aqueous 0 ✓ selected 96 solid 41 All/Clear ✓ properties Post-Calculate Post-Calculate Order Page Order ○ amount ○ fraction ○ activity										

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2. A convenient way to see the distribution of Fe for all values of <A> is to export the data into an Excel file

JactSage[™]





Ferrous Processing 19

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1. Because Fe gets distributed in the gas, metal and slag phases, all elements from these phases must be selected.

CodeSpeciesDataPhaseTVActivityMinimumMaximum160SolutionFToxid-PSEU0.29050.20411.000161SolutionFToxid-TiSp0.14974.2514E-020.1787162All ElementsGAS166All ElementsFTmisc-FeLQ167All ElementsFToxid-SLAGA#170All ElementsFToxid-SPINA171All ElementsFToxid-CORU173All ElementsFToxid-TiO2174All ElementsFToxid-ILMEA	CodeSpeciesDataPhaseTVActivity160SolutionFToxid-PSEU0.2905	Minimum Maxim	
160SolutionFT oxid-PSEU0.29050.20411.000161SolutionFT oxid-TiSp0.14974.2514E-020.1787162All ElementsGAS166All ElementsFT misc-FeLQ167All ElementsFT oxid-SLAGA#170All ElementsFT oxid-SPINA171All ElementsFT oxid-SPINA172All ElementsFT oxid-CORU173All ElementsFT oxid-TiO2174All ElementsFT oxid-ILMEA	160 Solution FToxid-PSEU 0.2905		uiii -
161SolutionFT oxid-TiSp0.14974.2514E-020.1787162All ElementsGAS </td <td></td> <td>0.2041 1.000</td> <td></td>		0.2041 1.000	
162 All Elements GAS Image: Constraint of the second	161 Solution FToxid-TiSp 0.1497	4.2514E-02 0.178	7
166 All Elements FTmisc-FeLQ Image: Comparison of the comparis	162 All Elements GAS		
167 All Elements FT oxid-SLAGA# Image: Constraint of the state of the st	166 All Elements FTmisc-FeLQ		
170 All Elements FT oxid-SPINA Image: Constraint of the second sec	167 All Elements FT oxid-SLAGA#		
171 All Elements FT oxid-Me0_A Image: Constraint of the state of the sta	170 All Elements FT oxid-SPINA		
172 All Elements FT oxid-CORU Image: Constant	171 All Elements FT oxid-MeD_A		
173 All Elements FT oxid-TiO2 174 All Elements FT oxid-IL MEA	172 All Elements FT oxid-CORU		
174 All Elements ET oxid-ILMEA	173 All Elements FT oxid-TiO2		
	174 All Elements FT oxid-ILMEA		
175 All Elements FT oxid-PSEU	175 All Elements FT oxid-PSEU		
		i i	



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3. Add columns to calculate the %Fe in each phase

0.00E+00

3.68E+01

that Fe in the slag is reduced as carbon is added

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7

5.00E-02 9.12E-05

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2.48E-04

0.00E+00

1.00E+02

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Calculating the liquidus of slag and metal: "Precipitate target" calculation



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1. As mentioned in slide 13, we will now calculate the equilibrium at 9.7g addition to reduce as much as possible the FeO content in the slag, but avoid pseudobrookite precipitation.

F Menu - Equilib: comments File Units Parameters Help		
	T(C) P(atm) Energy(J) Mass(g) Vol(litre)	III 🖳 🔁 😿
Reactants (2)	(gram) 100 FeTiO3 + <10A> C	
Products Compound species	- Solution species	Custom Solutions
, ⊊ gas	* + Base-Phase Full Name	0 fixed activities
aqueous 0	+ FTmisc-FeLQ Fe-lig	0 ideal solutions
pure liquids 0	I FToxid-SLAGA ASlag-lig all oxides + S	0 activity coefficients
* + pure solids 41	FToxid-SLAGG GSlag-liq with C/N/CN	Details
✓ suppress duplicates apply	FToxid-SLAG? ?Slag-liq	Beeudenume
* - custom selection	+ FToxid-SPINA ASpinel	Fseudonyms
species: 58	+ FToxid-Me0_A AMonoxide	apply List
	+ FToxid-CORU M203(Corundum)	E include meler velumes
	+ FToxid-TiO2 Rutile 🔽	
- none - Estimate T(K): 1000 Mass(g): 0	Legend I - immiscible 1 + - selected 8 solutions: 10 Select	<u>Total Species (max 1500)</u> 96 <u>Total Solutions (max 40)</u> 10 Default
Final Conditions	T(C) P(atm) Product H(J)	quilibrium
0.97	1675 1	transitions only
10 steps Table	1 calculation	open Calculate >>
FactSage 6.3 C:\FactS	ige\EguiCase3-1 DAT	

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We would now like to see if our temperature is well chosen. For this, we want to see what is the liquidus temperature of the slag and the metal.

 Press "Output" → "Stream File" → "Save solutions" and select the solution you would like to save. In this case, we want to save the metal and slag solutions.

2. In the pop-up window, enter the name of stream file

3. In the next window, enter any comments you might have.



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1. In the "Menu" window, we will select the liquid metal solution and all the solids as possible products.

		🕞 Menu - Equilib:	
		File Units Parameters Help	T(C) P(atm) Energy(J) Mass(g) Vol(litre)
		Reactants (1)	
			(gram) 100% [Liquid_Metal] 3 We will calculate only
		Products	the transitions.
		Compound species	or species
		gas 🛈 ideal 🔿 real 🛛 🔹	Base-Phase Full Name O fixed activities
		aqueous U	+ FTmisc-FeLQ Fe-liq 0 activity coefficients
		+ pure solids 41	FToxid-SLAGG GSlag-lig with C/N/CN
2 To make a	a	✓ suppress duplicates apply	FToxid-SLAG? ?Slag-liq
	a	* custom selection	FToxid-SPINA ASpinel
"cooling"		species: 41	FToxid-Me0_A AMonoxide
calculation w			FT oxid-TiD2 Butile
		Transitions - temperature	nd <u>Total Species (max 1500)</u> 47
will select		Number of	elected 1 Show Call C selected <u>Lotal Solutions (max 40)</u> 1
1675C as the	e	transitions: All	species: 6 Select
otorting	•		Default
starting		- Final Conditions	Equilibrium
temperature)	KA> KB>	T(C) P(atm) Product H(J) V normal C normal + transitions
and 1000C a		1675 1	1000 1 Stransitions only
	13	10 steps 🗖 Table	1+ calculations Calculate >>
the final			
temperature		FactSame C.2	
	-	racibage 6.3	



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1. In the "Results" F Results - Equilib 1674.17 C (page 1/27) Output Edit Show Pages window, it is seen 🗅 🗃 🔛 🚮 🚺 T(C) P(atm) Energy(J) Mass(g) Vol(litre) 111 🖳 🦰 😿 that Ti_3O_5 is ready 1310.89 C | 1241.54 C | 1209.12 C | 1456.26 C 1449.59 C 1449.13 C 1443.88 C 1443.5 C 1434.73 C 1432.91 C 1396.49 C 1394.32 C 1394.32 C 1354.54 C to precipitate at - 1674.17 C - 1516.99 C 1501.95 C 1500.71 C 1493.83 C 1492.88 C 1480.73 C 1479.94 C 1468.04 C 1467.38 C 1456.8 1674.17C (its FactSage 6.3 activity is 1). So (gram) 100% [Liquid Metal] = this is the liquidus 33.806 gram Fe-lig (33.806 gram, 0.61028 mol) temperature of our (1674.17 C, 1 atm, a=1.0000) (99.766 wt.% Fe FTmisc liquid metal. + 0.21705wt.% C FTmisc + 8.5413E-03 wt.% 0 FTmisc + 7.1498E-03 wt.% Ti FTmisc + 7.9054E-04 wt.% TiO FTmisc + 1.4588E-06 wt.% Ti20 FTmisc) System component Mole fraction Mass fraction 0.98960 0.99766 Fe Τi 8.9611E-05 7.7435E-05 n. 3.0258E-04 8.7395E-05 C 1.0010E-02 2.1705E-03 + 0 gram Ti305_solid-b FToxid (1674.17 C, 1 atm, S2, a=1.0000) 1310.89 C | 1241.54 C | 1209.12 C 2. At 1516.99C, 1456.26 C 1449.59 C 1449.13 C 1443.88 C 1443.5 C 1434.73 C 1432.91 C 1396.49 C 1394.32 C 1394.32 C 1354.54 C solid iron starts to 1674.17 C - 1516.99 C - 1501.95 C 1500.71 C 1493.83 C 1492.88 C 1480.73 C 1479.94 C 1468.04 C 1467.38 C 1456.8 precipitate. + 3.5331E-03 gram Ti305 solid-b FToxid (3.5331E-03 gram, 1.5801E-05 mol) (1516.99 C, 1 atm, S2, a=1.0000) + 0 gram Fe bcc FactPS (1516.99 C, 1 atm, S1, a=1.0000)



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1. An easier way to find the liquidus of the liquid metal solution is by using the "Precipitate target" calculation.

2. Right-click on
the Fe-liq selection
and select
"precipitate target
phase"

3. Leave the temperature field blank. This calculation will find the temperature at which the first solid will precipitate from the Fe-liq solution

F Menu - Equilib: File Units Parameters <u>H</u> elp		
☐ 😅 🔚 Reactants (1)	T(C) P(atm) Energy(J) Mass(g) Vol(litre)	M 📑 🔁
Solution FTmisc-FeLQ - clear	(gram) 100% [Liquid_Metal]	
 ✓ - all species * - custom select species m - merge dilute solution from → solution properties ✓ + - single phase 	Solution species * Base-Phase Full Name P FTmisc-FeLQ Fe-liq FToxid-SLAGA ASlag-liq all oxides + S FToxid-SLAGG GSlag-liq with C/N/CN FToxid-SLAG2 2Slag-liq	Custom Solutions 0 fixed activities 0 ideal solutions 0 activity coefficients Details
I - possible 2-phase immiscibility J - possible 3-phase immiscibility - standard stable phase ! - dormant (metastable) phase F - formation target phase	FToxid-SPINA ASpinel FToxid-MeO_A AMonoxide FToxid-CORU M203(Corundum) FToxid-TiO2 Rutile	Pseudonyms apply List
 P - precipitate target phase S - Scheil cooling target phase D - soliDification calculation C - composition target 	P - precipitate target species: 6 solutions: 1 Select	Default
Help	T(C) P(atm)	normal C normal + transitions transitions only open Calculate >>
FactSage 6.3		

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GactSage[™]

1. The liquidus temperature found is the same as in slide 23, but only one calculation had to be performed.

4	Results - E	quilib 1674.17 C				
0	utput <u>E</u> dit g	<u>s</u> how Pages				
ſ	🗅 🚘 🔛	DPT J	T(C) P(atm) Energy(J	I) Mass(g) Vol(litre)	111 🖳	• 🐺
1						
					Root Some 6	2
	(gram) 10	0% [Liquid_Metal] =			Factbage 6	
		and the second sec				=
	(33.806	gram #e-11q gram, 0.61028 mol)				
		(1674.17 C, 1 atm,	a=1.0000)			
		(99.766 wt.% Fe			FTmisc	
		+ 8.5413E-03 wt.% 0			FTMISC	
		+ 7.1498E-03 wt.% Ti			FTmisc	
		+ 7.9054E-04 wt.% TiO			FTmisc	
		+ 1.4588E-06 wt.% Ti20			FTmisc)	
		System component	Mole fraction	Mass fraction		
		Fe	0.98960	0.99766		
		Ti	8.9611 E -05	7.7435 E -05		
		0	3.0258E-04	8.7395E-05		
		C	1.00108-02	2.17058-03		
	+ 0	gram Ti305_solid-b			FToxid	
		(1674.17 C, 1 atm, S2,	a=1.0000)			
	+ 0	gram Fe bcc			T FactPS	
		(1674.17 C, 1 atm, S1,	a=0.92790)			
	+ 0	grom Ro fac			T Reat DG	
		(1674.17 C, 1 atm, S2,	a=0.91777)		I FACCED	
	+ 0	gram Ti407_solid	0 55060)		FToxid	
		(10/4.1/ C, 1 atm, SI,	a-0.00059)			×

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1. The same calculation can be performed on the liquid slag to find its liquidus temperature.

2. Select all the solids and FToxid solutions, because they can all precipitate out of the slag phase

F Menu - Equilib:						
		T(C) P(atm) Energy	(J) Mass(g) Vol(litre)	III 🖳 🕞 😿		
Reactants (1) (gram) 100% [Liquid_slag]						
Products						
Compound species	Solution s	pecies		Custom Solutions		
gas 💿 ideal 🔿 real 🛛 🛛	* +	Base-Phase	Full Name	0 fixed activities		
	IP	FToxid-SLAGA	ASlag-liq all oxides + S	0 ideal solutions 0 activity coefficients		
pure liquids U	+	FToxid-SPINA	ASpinel	Details		
* + pure solids 35	+	FToxid-MeO_A	AMonoxide	D'otalio		
suppress duplicates apply	+	FToxid-CORU	M203(Corundum)	- Pseudonyms		
* - custom selection	+	FToxid-TiO2	Rutile	apply List		
species: 35	+	FT oxid-ILMEA	Allmenite			
	+	FToxid-PSEU	Pseudobrookite	include molar volumes		
	+	FT oxid-TiSp	Titania_Spinel	Total Species (max 1500) 67		
Precipitate Larget FToxid-SLAGA Estimate T(C): 1000 Mass(g): 0	Legend – I - immisci P - precip + - selecti	ble 1 itate target ed 7	Show C all C selected species: 32 solutions: 9 Select	Total Solutions (max 40) 9 Default		
Final Conditions				Equilibrium		
(A) T(C) P(atm) Product H(J) O normal ransitions						
1 C transitions only						
10 steps Table 1 calculation C open Calculate >>						
FactSage 6.3						

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1. The results show that pseudobrookite will precipitate out at 1672.53C

2. The last two results show that our smelting temperature is quite close to both the metal and the slag liquidus temperatures. It would thus be wise to increase the smelting temperature, to avoid precipitation of solid phases.

	F Results - I	Equilib 1672.53 C				
	<u>O</u> utput <u>E</u> dit	<u>S</u> how Pages				
	D 😂 🖾	F F	T(C) P(atm) Energy(J) Mass(g) Vol(litre)	m 💷 ا	NT I
						^
		U	1.0000			
		System component	Mole fraction	Mass fraction		
		Fe	2.9184 E- 02	5.7594E-02		
		Ti	0.34944	0.59108		
		0	0.62138	0.35132		
I	+ 0	gren Deeudebrocki	ta V			
	1.0	(1672-53 C 1 atm	a=1.0000)			
		(1.5441 wt.% FeT	i205[2-]		FToxid	
		+ 49.898 wt.* Ti3	05[+]		FToxid	
		+ 1.6422 wt.% FeI	'i205		FToxid	
		+ 46.916 wt.% Ti3	05[-]		FToxid)	
		Site fraction of subl	attice constitue	nts:		
		Fe	3.0800 E- 02			
		TI3	0.96920			
			0 51540			
		TI3	0.48460			
		System component	Mole fraction	Mass fraction		
		fe Ti	3.84998-03 0.37115	7.68398-03 0.63494		
		2 \A/ith th		on at hand	it would bo	
		\mathbf{S} . with t	iis calculati	un at hanu,		
	+ 0	interesting t	o calculate	the viscosit	y of this slag.	
		<u>, 10.010</u> wo.o 112	-		FIOXIC	~

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Calculating the viscosity of the slag: "Viscosity" calculation



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Temperature-Pressure relationship at fixed slag composition: "Composition target" calculation



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Next, we would like to calculate the relationship between Temperature and partial pressure of oxygen at a constant slag composition.

	👍 Menu - Equilib: Ilmenite Smelting with variable carbo	F Composition Target 🛛 🗙		
	Eile Units Parameters Help T(C) P(atm) Energy(Reactants (2)	Solution 0X53-SLAGA Species Species composition Code numbers (97-100) FeD. Fe203, T(203)		
1. Select "composition target" for the slag phase.	(gram) 100 FeTiO3 Products Compound species + gas • ideal • real 17 + gas • ideal • real 0 + FTmisc-FeLQ - FTmisc-FeLQ	 log10 (species composition) element composition) log10 (element composition) species activity log10(species activity) 		
2. We will select 10% FeO as our composition target.		C - none (removes targets) - Values Enter a single value - or enter a range of values 'first last step' Species Fe0 0.1 mass fraction: (10%)		
	Estimate P(atm): 1.0 Mass(g): 0 C - composition target - species: Fe0	Cancel Help []		
3. Leave the Pressure field blank.	<a> T(C) P(atm) 0.97 1675 1725 1 10 10 steps Table	Product H(J) Froduct H(J) Frodu		
	FactSage 6.3 C:\FactSage\EquiCase3-1.DAT	li.		

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🕞 Results - Equilib 1675 C	, 15.3 atm (page 1/	51)			
Output Edit Show Pages Save or Print Image: state stat	T(C) P(atr Results peat Plot - weight % vs T(0	n) Energy(J) Mass(g) Vol(litre	1. We will p the	lot O ₂ activity versu temperature.	JS
Stream File	4 atr 1689 C 154 stm atm 7 Plot: log1	0 (activity) vs T(C)	C 154 store 1692 C 154 st		
Fact-Optimal	im 1 <u>File H</u> elp	100 FeTiO3 + <10A>	• C 🗸		
Fact-Function-Builder 🕨 ⁺ <	10A> Axes	Variables	Minimum	Maximum	
Refresh (1675 C, 15. (1675 C, 15. (0.99300 + 6.9874E-03 + 1.2508E-05 + 6.5063E-09 + 9.0519E-10 + 2.9778E-10 + 1.6771E-10 + 9.5294E-11 + 2.2086E-12 + 4.7483E-13 + 4.6477E-14 + 3.0038E-16 + 1.4998E-16 + 2.1111E-20	_ide	activity mole mole fract. gram weight % Alpha T(C) P(atm) Cp(J) G(J) Vol(litre) H(J) V(litre) S(J)	0 0 0 0 0 0 0 0 0 0 0 1675. 15.324 135.96 -1.2383E+06 0 -4.4970E+05 8.0069 394.72 1	15.496 1.2043 0.993139 55.108 98.925 0.97 1725. 15.603 138.05 -1.2187E+06 0 -4.4291E+05 8.1143 398.05 51	
+ 1.0934E-21 + 1.4294E-22 + 5.2688E-25 + 55.108 gram AS1	ag-1 FactSage 6.3	Species 1 selected Select Repeat C:\FactSage\Equi0.res	Graph Labels size: 9 no: 4 ♥ chemical ♥ integer # ♥ none	olay color full screen reactants O Viewer ile name O Figure Plot >> 6Feb13 51 sets	



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The graph shows that at lower temperatures, the oxygen pressure must be kept lower to keep the FeO content in the slag constant.



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Summarizing our findings:

9.7g C per 100g ilmenite seems to be ideal to reduce the amount of FeO in the slag while preventing the precipitation of pseudobrookite

The liquidus temperature of the resulting slag is 1672°C and the liquidus of the metal is 1674°C, so smelting at 1700°C would be better to avoid the precipitation of undesired phases



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