- Copper Extraction from Sulfide Concentrates
- Using Equilib Program
 - Selection of databases
 - Phase selection
 - ?Slag and ?Monoxide
 - Transition calculation
 - Export of results to Excel and plotting
- Phase Diagrams of Oxide Systems
 - In equilibrium with metals
 - At fixed or variable oxygen pressure
 - Being on a join





Copper Extraction from Sulfide Concentrates







Direct Smelting: Matte/Slag/Cu equilibrium

- Can all three phases Matte/Slag/Cu be in equilibrium?
- **Operating variables:**
 - Temperature
 - Oxygen pressure
 - Fe/SiO₂ ratio in the Slag
 - Amount of CaO in the Slag
- Subjects to examine:
 - Losses of Cu into Slag
 - Distribution of minor elements, Pb and Zn, among Matte, Slag and Cu
- Chemical system: Cu-Fe-Si-O-S + Ca-Pb-Zn
- Does this task make sense?
 - At T=const there are 4-2=2 degrees of freedom => fix $P(O_2)$, vary Fe/SiO_2
 - Study the effect of CaO at constant amount of CaO in the Slag
 - Pb(Slag)/Pb(Cu) will approach a constant as the amount of Pb approaches zero











Cu-S System







Selection of Databases



TDNucl - Thermodata nuclear database





FTmisc - FACT miscellaneous databases

- the system **S-Fe-Ni-Co-Cr**:

Liquid sulfide [FTmisc-MAT2] – from pure metal to pure sulfur Solid sulfide phases

- the matte smelting system **S-Cu-Fe-Ni-Co-Pb-Zn-As**:

Liquid matte [FTmisc-MATT] – liquid sulfide, does not extend to pure metal.

It is designed for calculation of matte / slag / metal equilibria

Consistent with FToxid-SLAG, FTmisc-CuLQ and FTmisc-PbLQ

It is not consistent with solid sulfide phases

- Liquid copper or speiss [FTmisc-CuLQ] – Cu-Pb-Zn-As-Fe-Ni-Au-S-O

- Liquid Fe [FTmisc-FeLQ] with dilute solutes AI, B, Bi, C, Ca, Ce, Co, Cr, Mg, Mn, Mo, N, Nb, Ni, O, P, Pb, S, Sb, Si, Te, Ti, V, W, Zn, Zr

- Liquid Pb [FTmisc-PbLQ] with dilute solues Ag, As, Au, Bi, Cu, Fe, Na, O, S, Sb, Sn, Zn





Selection of Databases

🖻 Data Se	earch					×
- Databases -	2/24 compour	nd databases, 2 SGTE	2/22 solution datab	ases —	cellane	ous
 □ ELEM □ FACT ☑ Fact53 ☑ FT oxid □ FT salt ☑ FT misc □ FT hall □ FT helg □ FT pulp □ FT lite 	<pre>FScopp FSlead FSlite FSstel FSupsi FSnobl Other OLIP OLIG</pre>	BINS BINS SGPS SGTE SGnobl SGsold SGnucl TDnucl OLIC OLIL	solutions only no data Clear All Select All Add/Remove Data RefreshDatabases	EXAM	SGSL	☐ SGTE*
- Options		de gaseous ions (pla aqueous species limited data comp	ismas) Dounds (25C)	.imits rganic species C inimum solution d	xHy, X(max) = components: O	2 1 ③ 2 cpts
Canc	el		Summary			OK





Input for Having Matte + Slag + Cu in Equilibrium

🕫 Reactants - Equ	rilib		
File Edit Table Unit	s Data Search H	Help	
D 🗃 🕂 🎹	T(C) P(atm)	Energy(J) Mass(g) Vol(litre)	111 💷 🔁
1 7			
1.571			1
Mass[n]	Species	Phase T(C)	P(total)** Stream# Data
100	Cu2S		
+ 100	Cu	_	1
+ <a>	FeO	_	1
+ <100-A>	SiO2	_	1
+ 0	CaO		1
+ 0.001	РЬ		1
+ 0.001	Zn	_	1
			Initial Conditions
FactSage 6.2 bet, Compound: 2/	24 databases Solution	2/22 databases	





Fixing Oxygen Pressure

4	Se	elec	tion - Equ	uilib	T(C) =	= 1	12	250 📘		
F	Eile	<u>E</u> dit	Show Sor	t						
0	ielect	ed: 38/3	8		GAS	So	rte	Page 20 🔺	Refresh	
	+	Code	Species	Data	Phase	Τ	۷	Activity		
	+	1	0(g)	FACT5	gas			5.4928E-10		
	+a	2	02(g)	FACT5	gas				📕 Fixed Partial Pressure 💦 🚺	Ś
	+	3	03(g)	FACT5	gas			3.3595E-21		-
	+	4	Si(g)	FACT5	gas			7.0399E-23	Cor for a range of values enter 'first last step') for	J
	+	5	Si2(g)	FACT5	gas			4.1834E-40	2 O2(g). Cancel	
	+	6	Si3(g)	FACT5	gas			3.1255E-55	Press [Cancel] if the partial pressure is no longer fixed.	-
	+	7	SiO(g)	FACT5	gas			2.8338E-11		-
	+	8	S(g)	FACT5	gas			7.4003E-08	14	
	+	9	S2(g)	FACT5	gas			1.9361E-06		
	+	10	S3(g)	FACT5	gas			2.6750E-11		
	+	11	S4(g)	FACT5	gas			1.1440E-15		
	+	12	S5(g)	FACT5	gas			7.4000E-21		
	+	13	S6(g)	FACT5	gas			1.4242E-24		
	+	14	S7(g)	FACT5	gas			1.5679E-28		
	+	15	S8(g)	FACT5	gas			3.0750E-33		
	Show	Selecter	d Select All	5	elect/Clear			Clear	οκ	
_	011044	Sciecter			Siccordical	_				





Selection of Stoichiometric Solids from FToxid

Eile	Edit	Show Sort			<u> </u>			ъ. 1
Selecte	ed: 55/19	U Uuplicates selecte	ed. <u> SUL</u>		rage		- neiles	41
+	Code	Species	Data	Phase	T	V	Activity	-
	194	Pb2Fe2O5(s)	FACT53	solid	T	0		
	195	Pb2FeSi2O7(s)	FACT53	pb-fe_melilite		0		
	196	Pb2Fe2Si2O9(s)	FACT53	melanotekite	T	0		
	197	Pb10Fe2Si2O17(s)	FACT53	solid	T	0		
	198	PbZnSiO4(s)	FACT53	solid	Т	0		
	199	Pb2ZnSi207(s)	FACT53	pb-zn_melilite	Т	0		_
	200	Pb8ZnSi6021(s)	FACT53	solid	Т	0		
+	201	SiO2(s)	FToxid	quartz(I)	Т	V	0.1004	
+	202	SiO2(s2)	FToxid	quartz(h)		V	0.3409	
+	203	SiO2(s3)	FToxid	tridymite(l)	Т	V	2.9347E-03	
+	204	SiO2(s4)	FToxid	tridymite(h)		V	0.3616	
+	205	SiO2(s5)	FToxid	cristobalite(I)	Т	V	1.3080E-02	
+	206	SiO2(\$6)	FToxid	cristobalite(h)		V	0.3612	
+	207	SiO2(\$7)	FToxid	coesite		V	0.1604	
+	208	SiO2(\$8)	FToxid	stishovite		V	1.7984E-03	
+	209	CaO(s)	FToxid	lime		V		





Selection of Solutions







Transitions

Results - Equilib A=1	IO (page 1/4) FactSage	e 6.2 be 📃 🗖 🔀
Output Edit Show Pages		
Image: A=10 A=63.2736 A=81.769 A=90	T(C) P(atm) Energy(J) Mass(g) Vol(litre)	<u>III 🤍 🖻</u> 🐼
+ 106.41 gram Cu-liq_or_spe (106.41 gram, 1.7060 mol)	riss	
(1250.00 C, 1 atm, (6.5704E-04 wt.* Pb	a=1.0000)	FTmisc
+ 98.087 wt.* Cu + 3.9339E-02 wt.* Fe + 1.9552 wt.* S]	FINISC FTNISC
+ 9.2040E-05 wt.* Zn + 1.7374E-02 wt.* 0	1	FTmisc FTmisc)
System component Pb	Mole fraction Mass fraction 1.9779E-06 6.5704E-06	

Check that the Matte and Cu phases contain the right amount of sulphur

ō	6.7732E-04	1.7374E-04		
+ 93.585 gram Matte				
(93.585 gram. 1.7542 mol)				
(1250.00 C. 1 atm.	a=1.0000)			
(19.389 wt. % S	_		FTmisc	
+ 0.57238 wt.% Fe	1		FTmisc	
+ 80.038 wt.* Cu			FTmisc	
+ 6.4079E-05 wt.% Zn			FTmisc	
+ 1.7725E-04 wt.% Pb			FTmisc)	
System component	Mole fraction	Mass fraction		
Dysocal components	4 56388-07	1 77258-06		
Zn	5 22798-07	6 40798-07		
Cu	0 67195	0 80038		
Fe	5 46788-03	5 72388-03		
s	0 32259	0 19389		
	0.02200	0.20000		
+ 15.437 gram ASlag-lig#1				
(15.437 gram, 0.21857 mol)				
(1250.00 C, 1 atm,	a=1.0000)			
(35.129 wt.* SiO2			FToxid	
+ 54.903 wt.* FeO			FToxid	
+ 5.4485 wt.% Fe20	3		FToxid	
+ 9.3912E-04 wt.% Pb0			FToxid	
+ 6.7716E-03 wt.% Zn0			FToxid	
+ 4.1536 wt.% Cu20			FToxid	
+ 0.14512 wt. % SiS2			FToxid	
+ 0.18082 wt.* FeS			FToxid	
+ 1.9091E-02 wt. % Fe2S	3		FToxid	
+ 2.70968-06 wt. * PbS	-		FToxid	
+ 2 1824R - 05 wt. $* 2nS$			FToxid	
+ 1.2435R-02 wt $* Cu2S$			FToxid)	
. 1.24002 02 0010 0425	-			~





A Series of Calculations

<u>File U</u> nits <u>P</u> arameters	<u>H</u> elp			
		T(C) P(atm) Energy	(J) Mass(g) Vol(litre)	M 🕒 🕒 🧏
Reactants (7)				
+ 100 Cu + <۵> FeO +	<100-65	SiD2 + 0.CaO	+ 0.001 Pb + 0.001 7	
	(100 A/	3/02 1 0 000	0.001110 1 0.001 21	<u>'</u>
Products				
Compound species	- Solution sp	ecies		Custom Solutions
∓ gas ⊙ ideal ⊂ real 38	* +	Base-Phase	Full Name 🔺	1 fixed activities
aqueous 0		FT oxid-SLAGA	ASlag-liq	0 ideal solutions
pure liquids 0		FT oxid-SLAGB	BSIag-liq	U activity coefficients
* ∓ pure solids 55		FToxid-SLAG?	?Slag-liq	Details
suppress duplicates apply	+	FT oxid-SPINA	ASpinel	- Recudenting
* - custom selection		FToxid-MeO_A	AMonoxide	rseudonyms
species: 93	. I	FToxid-Me0_?	?Monoxide	apply List
	<u> </u>	FT oxid-cPyr	Clinopyroxene	E include melar unbarre
	!	FT oxid-oPyr	Orthopyroxene	
_ Target	-Leaend-			Total Species (max 1500) 205
- none	I - immiscib	ole 1 💌	Show 🖲 all 🛛 selected	Total Solutions (max 40) 17
Estimate ALPHA: .6	! - dorman	12	species: 112	
Mass(q):	+ - selecte	d 3	solutions: 17 Select	
mass(g). jo				Default
Final Conditions				Equilibrium
<pre><a> </pre>	T(C)	P(atm)	▼ Product H(J) ▼	normal 🛛 normal + transitions
62.02.1	1250	1		transitions only 🔿 open
	1230	P.		predominant
10 steps I lable			20 calculations	Calculate >>





Output Results in Excel

Results - Equilib A=63 (page 1/20) FactSage 6.2 b 📃 🗖 🔀
<u>D</u> utput <u>E</u> dit <u>S</u> how Pages
T(C) P(atm) Energy(J) Mass(g) Vol(litre)
$\mathbf{x} = 63$ $\mathbf{x} = 64$ $\mathbf{x} = 65$ $\mathbf{x} = 66$ $\mathbf{x} = 67$ $\mathbf{x} = 69$ $\mathbf{x} = 70$ $\mathbf{x} = 71$ $\mathbf{x} = 73$ $\mathbf{x} = 74$ $\mathbf{x} = 75$ $\mathbf{x} = 76$
A-05 A-05 A-05 A-05 A-05 A-05 A-16 A-11 A-12 A-15 A-15 A-16
(gram) 100 Cu2S + 100 Cu + <a> FeO + <100-A> SiO2 +
(gram) = 0 Ca0 + 0.001 Pb + 0.001 Zp =
+ 0.81356 02
(12) Page Range Type of Output
(5. • All 20 pages
+ 2 + 1 C Current page 1 C Text file (*.txt)
+ 1. C Equilib Results File (Equi*.res)
+ 2.
+ 1. • Excel Spreadsheet
+ 1. C Open Text Spreadsheet Spreadsheet setup
+ 7
+ 1. 🔽 Swap rows & columns
+ 1.
+ 1 + 5 Cancel
+ 1
+ 5.4928E-10 0 FACT53
+ 3.1404E-10 Fe0 FACT53
+ 7.8362E-11 Si0 FACT53
+ 4.9120E-11 FeS FACT53 🗸





Select Species for Output

Output Edit Show Pages Image: Show Pages T(C) P(atm) Energy(J) Mass(g) Vol[litre) Image: Show Pages A=77 A=78 A=79 A=80 A=81 A=82 A=63 A=64 A=65 A=66 A=67 A=68 A=69 A=70 A=71 A=72 A=73 A=74 A=75 A=76 (gram) 100 Cu2S + 100 Cu + <a> Fe0 + <100-A> Si02 + Image: Species Setup Image: Species Properties Image: Species Properties Image: Species Properties Image: Species Properties Image: Species Setup Image: Species Setup
Image: Column: -12 - Variable: Columns: -7 - 2 - 2 - 2 - 2 - 2 - 2 - 2 - 2 - 2 -
A=77 A=78 A=79 A=80 A=81 A=82 A=63 A=64 A=65 A=66 A=67 A=68 A=69 A=70 A=71 A=72 A=73 A=74 A=75 A=76 (gram) 100 Cu2S + 100 Cu + <a> Fe0 + <100-A> Si02 + (gram) 0 Ca0 + 0.001 Pb + 0.001 Zn = + 0. Spreadsheet Setup X 0. System Properties Property columns 2 - - X 0. Species Properties Column: -1 - -2 - - - - - Columns - - - Columns - - - Columns - - - Columns - <t< td=""></t<>
A=63 A=64 A=65 A=66 A=67 A=68 A=69 A=70 A=71 A=72 A=73 A=74 A=75 A=76 (gram) 100 Cu2S + 100 Cu + <a> Fe0 +
(gram) 100 Cu2S + 100 Cu + <a> FeO + <100-A> SiO2 + (gram) 0 CaO + 0.001 Pb + 0.001 Zn = + 0. Spreadsheet Setup 0. System Properties Property columns 2 → Column: 1. · 2. Variable: Alpha T(C) Species Properties Columns per species 1 → C order species • order props. Columns 7
(gram) 0 Ca0 + 0.001 Pb + 0.001 Zn = + 0. Spreadsheet Setup 0. System Properties Property columns 2 ↓ Column: 1- 2- Variable: Alpha T(C) Species Properties Columns per species 1 ↓ C order species • order props.
(gram) 0 ca0 + 0.001 ps + 0.001 zn = + 0.: Spreadsheet Setup 0.: System Properties Column: .12. Variable: Alpha T(C) Species Properties Columns per species 1 Corder species • order props.
+ 0. Spreadsheet Setup 0. System Properties Property columns 2 + Column: -12 - Variable: Alpha T(C) Species Properties Columns per species 1 + C order species © order props.
0. System Properties Property columns 2 Column: ·1 · · · · · · · · · · · · · · · · · ·
Property columns 2 + Column: -12 - Variable: Alpha T(C) Species Properties Columns per species 1 + C order species • order props. Columns: 7
Column: · 1 · · 2 · Variable: Alpha T(C) Species Properties Columns per species Columns: 7 Columns per species 1 • O order species • order props.
Variable: Alpha T(C) Species Properties Columns: Columns: 7 Columns per species 1 Corder species Order props. Columns: 7
Species Properties Species Columns: 7 Columns per species 1 Corder species Corder props.
Species Properties Species Columns: 7 Columns per species 1
Species Properties Columns per species Columns: 7 Columns per species I <t< td=""></t<>
Columns per species 1 - Corder species Corder props.
Capacity Capacity
Variable: Wt% Default
Species: 5
+ 3 1404E-10 E=0 E0CT53
+ 2.2758E-10 Cu0 FACT53
+ 7.8362E-11 SiO FACT53 + 4.9120E-11 FeS FACT53





₽ S	prea	dsheet -	Equilit	o T(C) =	= 1		×									
File	Edit	Show														
_	_	_														
Selec	ed: 5/225		Spreadshe	et Species	Page 1	- Refres	sh g	2								
	Code	Coocies	Data	Phase	TV	Activitu										
-	LOUE	Shecies	Data	Гпазе		Activity										
+	272	Pb(Cul Q)	ETmise	ETmise-Cul Q		5 1975E-06										
	273		FTmisc	FTmisc-CuLQ		0.9767										
	274	Fe(CuLQ)	FTmisc	FTmisc-CuLQ		6.2170E-03										
	275	S(CuLQ)	FTmisc	FTmisc-CuLQ		8.4239E-05	-	F S	brea	dsheet -	Eauilit	5 T(C)	= 1			X
	276	Zn(CuLQ)	FTmisc	FTmisc-CuLQ		1.8842E-08						1 ()				لععار
	277	O(CuLQ)	FTmisc	FTmisc-CuLQ		4.3782E-05		Eile	<u>E</u> dit	Show						
										n.			Deer	1		- -
	286	S(MATT)	FTmisc	FTmisc-MATT		8.3687E-05		Selec	ted: 5/225	<u>'</u>	Spreadshe	et Species	Fage	<u> </u>	- neite	asin <u>o</u>
	287	Fe(MATT)	FTmisc	FTmisc-MATT		6.2170E-03		+	Code	Species	Data	Phase	Т	V	Activitu	
	288	Cu(MATT)	FTmisc	FTmisc-MATT		0.6014		<u> </u>	509	All Elements		ETmisc-MAT	T		nounty	
	289	Zn(MATT)	FTmisc	FTmisc-MATT		1.8842E-08		+	520	All Elements		FToxid-SLAG	GA#1			
+	290	Pb(MATT)	FTmisc	FTmisc-MATT		5.1978E-06			523	All Elements		FT oxid-SPIN	A			
									525	All Elements		FToxid-MeO	?			
+	313	Si02(SLAGA)	FToxid	FToxid-SLAGA		0.8350	τl		526	All Elements		FToxid-cPyr				
	314	CaO(SLAGA)	FToxid	FToxid-SLAGA			<u> </u>		527	All Elements		FToxid-oPyr				
L		he Species Preper	tion on defined	in the Coreadah	act Colum	1			528	All Elements		FToxid-WOL	LA			
[+0	enotes all t	ine species Floper	ues as denned	in the spreadsh	eet setup.]			529	All Elements		FT oxid-bC2S	i			
									530	All Elements		FT oxid-aC2S	i			
		Select All	Clea	16	OK				531	All Elements		FToxid-Mel_				
									532	All Elements		FToxid-OlivA				
									533	All Elements		FT oxid-ZNIT				
									534	All Elements		FT oxid-WILL	-			_
									535	All Elements		FT oxid-PbO_	_			_
									536	All Elements		FT oxid-PCSi				
									onotoo all	the Creation Proce	rtice as defined	in the Core of	aboot S al	hum.		
								[+0	enotes all	une opecies mope	aues as denned	in the spread	srieet pe	tup.		
											1				1	
										Select All	Cle-	ar _	0	ĸ		





Cu losses to Slag







Distribution of Pb between Slag and Cu







Distribution of Pb between Slag and Matte







Cu losses to Slag







Distribution of Pb between Slag and Cu







Distribution of Pb between Slag and Matte









GactSage™



F Components	- Phase Diagram	
<u>Eile Edit Units Da</u>	ata Search <u>H</u> elp	
D 🖻 +	T(C) P(atm) Energy(J) Mass(mol) Vol(litre)	M 📑 🔂
1.2		
	Components	
	Fe	
	0	
	Next >>	
FactSage 6.2 bet Compound:	3/24 databases Solution: 2/22 databases	





Bact	Bact Sage"	SATE		Mise	ellane	ous
 ELEM FACT Fact53 FT salt FT salt FT misc FT hall FT helg FT pulp FT lite 	☐ FScopp ☐ FSlead ☐ FSlite ☑ FSstel ☐ FSupsi ☐ FSnobl Other ☐ OLIP ☐ OLIG	BINS BINS SGPS SGTE SGnobl SGsold SGnucl TDnucl OLIC OLIL	compounds only solutions only no data Clear All Select All Add/Remove Data RefreshDatabases		SGSL	SGTE*

	Selection - Equilib						
	<u>Eile E</u> dit	: Show Sort					
	Selected: 5/18	B Duplicates select	ted. SO	LID	d by Code	•	
F Menu - Phase Diagram: Fe-O phase diagra	r + Cod	e Species	Data	Phase	TV	Activity	-
File Units Parameters Variables Help	15	Fe2U3(s2) Fe2U3(s3)	FACT53	high-pressure-he	V		
	17	Fe304(s)	FACT53	magnetite	V		
I(C) P(atm) Energy(J) Mass(moi) Vol(litre)	18	Fe304(s2)	FACT53	magnetite	V		
Components (2)	19	Fe304(s3)	FACT53	high-pressure-m	V		
· · · · ·	20	Fe304(s4)	FACT53	high-pressure-m	V		
Fe + O	+ 21	Fe(s)	FSstel	bcc_a2			
	+ 22	Fe(s2) Fe(202(a)	FSstel ESstel	ICC_al bematite	V		
- Products	- 23	Fe304(s)	ESstel	magnetite	V		
Compound species Solution species	- 25	Fe304(s2)	FSstel	magnetite	V		
Figas € ideal C real 5	+ 26	Fe2O3(s)	FToxid	hematite	V		
aqueous 0 + FSstel-FE-L Fe-LIQUID	+ 27	Fe2O3(s2)	FToxid	high-pressure-he	V		
pure liquids 0 I FToxid-SLAGA ASlag-liq	+ 28	Fe2O3(s3)	FToxid	high-pressure-he	V		
* pure solids 5 + FToxid-SPINA ASpinel							
suppress duplicates apply + FToxid-MeO_A AMonoxide							
* - custom selection							
species: 10	Show Sele	cted Select All	Select/	Clear Cl	ear	OK	
	inclu	ude molar volumes					
	Total Sp	<u>becies (max 1500)</u> 24					
- none - Legend Vision Show I all C selecte	ed <u>Total So</u>	olutions (max 40) 5	;				
Estimate T(K): 1000 + selected 3 second							
Massfreelt 0	st _						
		Default					
Variables	Phase Dia	aram					
T(C) 0/(Fe+0)	1	_					
400 1800 0 1							
, , , , , , , , , , , , , , , , , , , ,	×						
T(C) vs O/(Fe+O)		Calculate >>					
FactSage 6.2 beta g:\CAD\\metall-saturated\PhasFe-0_1atm.DAT							
			110				















GactSage[™]









P=10000 atm













Components - Phase Diagram	
Eile Edit Units Data Search Help T(C) P(atm) Energy(J) Mass(mol) Vol(N	itre)
Components	
Zn	🗖 Data Search 🔀
	Databases - 3/24 compound databases, 2/22 solution databases Cact GattSage" SGTE ELEM FScopp BINS FACT FSlead SGPS FactS3 FSlite SGTE FactS3 FSlite SGTE FToxid FSstel SGnobl FTsalt FSupsi SGsold Select All Select All
	FThall FThelg Other TDnucl FThelg OLIP OLIC FTlite OLIG OLIL Information -
	Click on a box to include (or exclude) a database in the data search. Normally databases are 'coupled' - that is both the compound and solution database (when available) will be selected. To 'uncouple' a databases click-mouse-right-button (note, this is NOT recommended).
Next >> FactSage 6.2 bet. Compound: 3/24 databases Solution: 2/22 databases	Options Include □ gaseous ions (plasmas) Organic species CxHy, X(max) = 2 □ aqueous species Minimum solution components: ○ 1 ○ 2 cpts
	Cancel Summary OK





	Selection - Equilib	
	Eile Edit Show Sort	
	Selected: 7/23 Duplicates selected.	OLID Sorted by Code
	+ Code Species Data	Phase T V Activity
Menu - Phase Diagram: Only O2 gas species is se	25 Fe3U4(s4) FAC15 26 Zn(s) FACT5	3 high-pressure-m V 3 solid
Eile Units Parameters Variables Help	27 ZnO(s) FACT5	3 zincite
	28 ZnFe2D4(s) FACT5:	3 solid
T(C) P(am) Energy(J) Mass(moi) Vol(ine)	+ 30 Fe(s2) FSstel	fcc_a1
Components (3)	31 Fe2D3(s) FSstel	hematite V
	32 Fe3U4(s) FSstel 33 Fe3O4(s2) FSstel	magnetite V magnetite V
Fe + Zn + O	+ 34 Zn(s) FSstel	hcp_zn o
	+ 35 Fe203(s) FToxid	hematite V
- Products	+ 36 Fe2O3(s2) FToxid	high-pressure-he V
Compound species Solution species	+ 37 Fe203(\$3) FT0Xid + 38 Zn0(\$) FT0Xid	zincite
* ∓ gas 🖲 ideal O real 1 🔹 + Base-Phase Full Name 🔺 0 fix		
aqueous 0 + FSstel-FEZ1 FEZN4 0 id		
pure liquids 0 + FSstel-FEZ2 FEZN_DELTA 0 ad		
* + pure solids 7 + FSstel-FEZ3 FEZN_ZETA	Show Selected Select All Select	/Clear Clear OK
suppress duplicates apply + FSstel-HCP HCP_A3:Me2(C,N)		
* custom selection I FToxid-SLAGA ASlag-liq		
species: 8 + FToxid-SPINA ASpinel apply	List	
+ FToxid-MeD_A AMonoxide	lude moler volumes	
+ FToxid-ZNIT Zincite 🔽 Testal (Capacias (may 1500) 50	
	Colutions (may 40) 14	
I immiscible 1		
Estimate T(K): 1000 + - selected 12 species: 51 Select		
Mass(mol): 0 solutions: 14	Default	
	Dordan	
Variables Phase Di	agram	
T(C) 0/(Fe+Zn+0) Zn/(Fe+Zn+0) A		
	Calculate >>	
[A=0, B=Fe, C=2n]		
FactSage 6.2 beta g:\\PhasFe-Zn-0_1500-C_02-gas.DAT	//	







FactSage[™]

Oxides and Pyrometallurgy 35

2010








F Components - Phase Diagram	
Eile Edit Units Data Search Help T(C) P(atm) Energy(J) Mass(mol) Vol(litre 1-2 Image: Search Image: Search	
Fe0	E Data Soarch
	Date Sear CII Date Sear CII Databases - 1/24 compound databases, 1/22 solution databases Date Sear Clark Searce Searce Searce Compounds only Searce
Next >> FactSage 6.2 bet Compound: 1/24 databases Solution: 1/22 databases	Options Include Limits Default gaseous ions (plasmas) Organic species CxHy, X(max) = 2 Minimum solution components: ○ 1 ④ 2 cpts Cancel Summary





🕫 Menu - Phase Diagram: last system	
<u>Eile U</u> nits <u>P</u> arameters <u>V</u> ariables <u>H</u> elp	
🗈 🚘 🔚 T(C) P(atm) Energy(J) Mass(mol) Vol(litre)	M 🖳 🔁 🛪
Components (2)	
FeO + ZnO	
Products	
Compound species Solution species	Custom Solutions
gas (© ideal (C) real U * + Base-Phase Full Name	0 ideal solutions
pure liquids 0 + FT oxid-SPINA ASpinel	0 activity coefficients
+ pure solids 4 + FToxid-MeO_A AMonoxide	Details
suppress duplicates apply + FToxid-ZNIT Zincite	- Pseudonyms
species: A	apply 🗖 List
	I include molar volumes
Target Legend Fair Charles Charles	Total Species (max 1500) 28
I - inmiscible 1 I Show to all to selecte	
Estimate I (K): 1000 +- selected 3 species: 24 Selected 3	st
Mass(mol): 0 solutions: 5	Default
Variables	Phase Diagram
T(C) ZnO/(FeO+ZnO)	Y
800 2000 0 1	
	Calculate >>
FactSage 6.2 beta	1





Variables: FeO-ZnO T(C) vs composition #1.



















FeO-ZnO System (oxide phases and pure Fe)

F Menu - Phase Diagram: Metal phases are not se	elec	🕫 Select	tion - Equil	ib			
File Unite Darameters Variables Help		<u>E</u> ile <u>E</u> dit	Show Sort				
<u>Energianeters vanables Elep</u>		Selected: 6/17	Duplicates selected	. SOLID	Sorted	by Code	
I C P(atm) Energy(J) Mass(mol) Vol(litre)	ļ	+ Code	Species	Data	Phase	TV	Activity
Components (2)		+ 13	Fe(s)	FACT53 b	cc		riotrity
		+ 14	Fe(s2)	FACT53 fo	50 		
FeO + ZnO		15	FeU(s) Fe2O2(a)	FACT53 W	vustite ematite	V	
		17	Fe2O3(s)	FACT53 h	igh-pressure	V	
- Products		18	Fe2O3(s3)	FACT53 h	igh-pressure	V	
Compound species Solution species	ustom Solutio	19	Fe304(s)	FACT53 m	hagnetite	V	
Composing species	0. fived activit	20	Fe3U4(s2) Fe3U4(s3)	FACI53 m	iab-pressure-		
	0 ideal solutio	22	Fe304(s3)	FACT53 h	igh-pressure	V	
* pure liquids 1 + ETavid SDNA ASiaghiq	0 activity cos	23	Zn(s)	FACT53 s	olid		
* pure solids 6 + FToxid-SFTNA Appiner	[24	ZnO(s)	FACT53 z	incite		
The solids of the provide the solid solution of the provide the solid solution of the solid so		25	ZnFe204(s)	FACT53 s	olid omatika		
F Suppress duplicates apply	seudonyms-	+ 27	Fe203(s) Fe203(s2)	FToxid h	iah-pressure	V	
- custom selection	apply 🗖	+ 28	Fe2O3(s3)	FToxid h	igh-pressure	V.	
species. 7		+ 29	Zn0(s) _	FToxid z	incite		
	include mo						
	E Sala	ction -	Fauilib				
- none - I - immiscible 1 🔽 Show 👁 all O selected	- Jele		Equilib		l		
Estimate T(K): 1000 +-selected 3 species: 24 or 1	<u>Eile E</u> d	it Show	Sort				
Mass(mol): 0 solutions: 5 Select	Colored 1.0				Cashad bu	Carla	
	Selected: 17	b] Dupilcates	selected. LIQU		Sorred by	Loge	
Variables Pha	+ Cod	le Spec	cies Data	Pha	ase T	V A	ctivity
T(C) ZnU/(FeU+ZnU)	+ 7	Fe(liq)	FACT5	3 liquid			
800 2000 01	8	FeO(liq)	FACT5	3 liquid			
	9	Fe304(liq)	FACT5	3 liquid			
[[T(C) vs ZnD/[FeO+ZnD]]	10	Zn(liq)	FACT5	3 liquid			
	11	ZnO(liq)	FACT5	3 liquid			
FactSage 6.2 beta g:\\Phashe-Zn-U_FeU-ZnU_no-he2U3.DA1	12	ZnO(liq)	FToxid	liquid			
						_	
	w Selected	Select Al	Select/Cle	ear	Clear		OK











FeO-ZnO System (oxide phases and pure Fe)







F Components - Phase Diagram	
Eile Edit Units Data Search Help T(C) P(atm) Energy(J) Mass(mol) Vol	(litre)
1 · 3	▪ Data Search
Fe	Databases - 2/24 compound databases, 2/22 solution databases Image: Compound Solutions only Image: Compound Solutions only Image: Fact Image: Fact
	<u>Oxide phases</u> Metal phases from FSstel
Next >> FactSage 6.2 bet Compound: 2/24 databases Solution: 2/22 databases	Options Include gaseous ions (plasmas) Organic species CxHy, X(max) = 2 Minimum solution components: ○ 1 ○ 2 cpts
	Cancel Summary OK





Menu - Phase Diagram: Correct phase diagram	n Fe 💶 🗖 🗙		
File Units Parameters Variables Help		1	
T(C) P(atm) Energy(J) Mass(mol) Vol(litre)	TH 🖦 🦱 🐨		
Lomponents [3]			
FeO + ZnO + Fe			
Products			
Compound species Solution species	- Custom Solutions		
aqueous 0 + Esstel-FFZ1 FEZNA	0 ideal solutions		
pure liquids 0 + FSstel-FEZ2 FEZN_DELTA	0 activity coefficients		
* pure solids 7 + FSstel-FEZ3 FEZN_ZETA	Details		
suppress duplicates apply + FSstel-HCP HCP_A3:Me2(C,N)	F Selection - Equ	uilib	
*- custom selection I FT0xid-SLAGA AStag-liq species: 7 + FT0xid-SPINA AStag-liq	File Edit Show Sor	+	
+ FToxid-MeD_A AMonoxide	Life Fair Show Sol	<u>L</u>	
+ FToxid-ZNIT Zincite 💌	Selected: 7/10 Duplicates select	ed. SOLID Sorted	d by Code
Legend	+ Code Species	Data Phase	T V Activity
Estimate T(K): 1000 +- selected 12 species: 51	+ 5 Fe(s)	FSstel bcc_a2	
Mass(mol): 0 Select	\pm 6 Ee(c2)	TO ALL GAR AT	
		Fostel Icc_al	
	7 Fe203(s)	FSstel fcc_al FSstel hematite	V
Variables	7 Fe2O3(s) 8 Fe3O4(s) 9 Fe3O4(s2)	FSstel hematite FSstel magnetite FSstel magnetite	V
Variables Pha T(C) Zn0/(Fe0+Zn0+ Fe/(Fe0+Zn0+Fe)	7 Fe2O3(s) 8 Fe3O4(s) 9 Fe3O4(s2) + 10 Zn(s)	FSstel hematite FSstel magnetite FSstel magnetite FSstel hcp_zn	V
Variables Pha T(C) Zn0/(Fe0+Zn0+ Fe/(Fe0+Zn0+Fe Y 800 2000 0 1 0.001 Y	7 Fe2O3(s) 8 Fe3O4(s) 9 Fe3O4(s2) + 10 Zn(s) + 11 Fe2O3(s)	FSstel hematite FSstel magnetite FSstel magnetite FSstel hcp_zn FToxid hematite	
Variables Pha T(C) ZnD/(Fe0+Zn0+ Fe/(Fe0+Zn0+Fe) Y 800 2000 0 1 0.001 Y T(C) vs ZnD/(Fe0+Zn0+Fe) Y Y	7 Fe2O3(s) 8 Fe3O4(s) 9 Fe3O4(s2) + 10 Zn(s) + 11 Fe2O3(s) + 12 Fe2O3(s2) + 12 Fe2O3(s2)	F3stel rcc_al FSstel hematite FSstel magnetite FSstel hcp_zn FToxid hematite FToxid high-pressur FToxid high-pressur	
Variables Pha T(C) Zn0/(Fe0+Zn0+ Fe/(Fe0+Zn0+Fe Y 800 2000 0 1 0.001 Y Y T(C) vs Zn0/(Fe0+Zn0+Fe) Y Y	7 Fe2O3(s) 8 Fe3O4(s) 9 Fe3O4(s2) + 10 Zn(s) + 11 Fe2O3(s) + 12 Fe2O3(s2) + 13 Fe2O3(s3) + 14 Zn(s)	F3stel rcc_a1 FSstel hematite FSstel magnetite FSstel hcp_zn FToxid hematite FToxid high-pressur FToxid high-pressur FToxid zincite	
Variables Pha T(C) ZnD/(Fe0+Zn0+ Fe/(Fe0+Zn0+Fe) Y 800 2000 0 1 0.001 Y T(C) vs ZnD/(Fe0+Zn0+Fe) Y FactSage 6.2 beta g:\\PhasFe-Zn-0_Fe0-Zn0-Fe_using-FSstel.DAT	7 Fe203(s) 8 Fe304(s) 9 Fe304(s2) + 10 Zn(s) + 11 Fe203(s) + 12 Fe203(s2) + 13 Fe203(s3) + 14 Zn0(s)	FSstel Icc_al FSstel hematite FSstel magnetite FSstel hcp_zn FToxid hematite FToxid high-pressur FToxid zincite	V V V V V V V
Variables Pha T(C) Zn0/(Fe0+Zn0+ Fe/(Fe0+Zn0+Fe Y 800 2000 0 1 0.001 Y T(C) vs Zn0/(Fe0+Zn0+Fe) Y FactSage 6.2 beta g:\\PhasFe-Zn-0_Fe0-Zn0-Fe_using-FSstel.DAT	7 Fe2O3(s) 8 Fe3O4(s) 9 Fe3O4(s2) + 10 Zn(s) + 11 Fe2O3(s) + 12 Fe2O3(s2) + 13 Fe2O3(s3) + 14 ZnO(s)	F3stel fcc_a1 FSstel hematite FSstel magnetite FSstel hcp_zn FToxid hematite FToxid high-pressur FToxid high-pressur FToxid zincite	V V V V V V V
Variables Pha T(C) ZnD/(Fe0+Zn0+ Fe/(Fe0+Zn0+Fe) Y 800 2000 0 1 0.001 Y T(C) vs ZnD/(Fe0+Zn0+Fe) Y FactSage 6.2 beta g:\\PhasFe-Zn-0_Fe0-Zn0-Fe_using-FSstel.DAT Oxide phases	7 Fe2O3(s) 8 Fe3O4(s) 9 Fe3O4(s2) + 10 Zn(s) + 11 Fe2O3(s) + 12 Fe2O3(s2) + 13 Fe2O3(s3) + 14 ZnO(s)	F3stel fcc_a1 FSstel hematite FSstel magnetite FSstel hcp_zn FToxid hematite FToxid high-pressur FToxid high-pressur FToxid zincite	
Variables Pha T(C) Zn0/(Fe0+Zn0+ Fe/(Fe0+Zn0+Fe) 800 2000 0 1 0.001 T(C) vs vs T(C) vs vs State gs vs FactSage 6.2 beta gs vs Oxide phases Metal phases from FSstel	7 Fe2O3(s) 8 Fe3O4(s) 9 Fe3O4(s2) + 10 Zn(s) + 11 Fe2O3(s) + 12 Fe2O3(s2) + 13 Fe2O3(s3) + 14 ZnO(s)	FSstel rcc_a1 FSstel hematite FSstel magnetite FSstel hcp_zn FToxid hematite FToxid high-pressur FToxid high-pressur FToxid zincite	ear OK











FeO - ZnO - Fe



mole Fe/(FeO+ZnO+Fe) = 0.001





FeO-ZnO in Equilibrium with Metals vs FeO-ZnO

FeO - ZnO - Fe









– Databases	- 2/24 compour	nd databases,	2/22 solution data	Jases —	
Fact	GactSage"	SGTE	compounds only	Miscellan	eous
 □ ELEM □ FACT □ Fact53 □ FT oxid □ FT salt □ FT misc □ FT hall □ FT helg □ FT pulp □ FT lite 	 FScopp FSlead FSlite FSstel FSupsi FSnobl Other OLIP OLIF 	 BINS SGPS SGTE SGnobl SGsold SGnucl TDnucl OLIC OLIC 	solutions only no data Clear All Select All Add/Remove Data RefreshDatabases	EXAM D SGSL	. □ SGTE*
			<u>Oxide pha</u> <u>Metal pha</u>	<u>ases</u> ises from SGTE	
– Options Defau	lt □	de gaseous ions (pl aqueous specie: limited data com	asmas) s pounds (25C)	Limits Drganic species CxHy, X(max Minimum solution components: (i) = 2 ⊃ 1 ⊙ 2 cpts
					,

🕫 Menu - Phase D	iagram: Correct phase diagrar	n Fe 💶 🗖 🔀	
Eile Units Parameters	<u>V</u> ariables <u>H</u> elp		
Components (3)	T(L) P(atm) Energy(J) Mass(mol) Vol(litre)	III 🕒 🕒 🕱	
	FeO + ZnO + Fe	Selection - Equilib	
Desidents		Eile Edit Show Sort	
Compound species	Solution species	Selected: 7/7 SOLID	Sorted by Code
gas ideal Creal 0 aqueous 0		+ Code Species Data + 6 Fe2D3(s) FToxid	Phase T V Activity
pure liquids 0	+ FToxid-SPINA ASpinel	+ 7 Fe2O3(s2) FToxid	high-pressur V
y suppress duplicates apply	+ FToxid-MeU_A AMonoxide + FToxid-ZNIT Zincite	+ 8 Fe2U3(s3) FToxid + 9 ZnO(s) FToxid	zincite
species: 7	+ SGTE-LIQU LIQUID + SGTE-ECC1 ECC 41	+ 10 Fe(s) SGTE + 11 Fe(s2) SGTE	bcc_a2 o
	+ SGTE-BCC1 BCC_A2	+ 12 Zn(s) SGTE	hcp_zn o
-Target	Legend		
- none - Estimate T(K): 1000	I - immiscible 1 I Show to all to selected + - selected 11 species: 51	w Calastad Calastall Calastall	Chan DV
Mass(mol):	solutions: 13 Select	ow selected select All select/Liear	
Variables		ase Diagram	
T(C) Zn0/(Fe0+Zn0-	+ Fe/(Fe0+Zn0+Fe		
		X Calculate XX	
T(C) vs Zn0/(Fe0+Zn0+Fe)			
FactSage 6.2 beta g:\\Ph	asFe-Zn-0_Fe0-Zn0-Fe_SGTE.DAT		
		<u>Oxide pha</u>	<u>ses</u>

Metal phases from SGTE

CRC1

Montreal

2010



FeO - ZnO - Fe



mole Fe/(FeO+ZnO+Fe) = 0.001





FeO-ZnO in Equilibrium with Metals (FSstel vs SGTE)

FeO - ZnO - Fe

mole Fe/(FeO+ZnO+Fe) = 0.001



Montreal

2010

	2/24 compour	nd databases, 1	1/22 solution datab	ases —		
Gact	GactSage"	SGTE	compounds only	Mise	cellane(ous
 □ ELEM □ FACT ☑ Fact53 ☑ FT oxid □ FT salt □ FT misc □ FT hall □ FT helg □ FT pulp □ FT lite 	 FScopp FSlead FSlite FSstel FSupsi FSnobl Other OLIP OLIG 	BINS BINS SGPS SGTE SGnobl SGsold SGnucl TDnucl OLIC OLIL	solutions only no data Clear All Select All Add/Remove Data RefreshDatabases	EXAM	SGSL	□ SGTE*
	<u>Ox</u> <u>St</u>	de	etric metal p	<u>hases fro</u>	m Fact5	3
- Options Defau		aqueous species	amas)	finimum solution c	omponents: O	1 🖸 2 cpts



👎 Menu - Phase Diagram: FeO-ZnO in equilibrium	wi	Selection -	Equilib	
File Unite Darameters Variables Help		<u>E</u> ile <u>E</u> dit Show	Sort	
		Selected: 6/17 Duplicates	selected. SOLID So	orted by Code
L C Flami Energy() Mass(mol) Vollide)	111	+ Code Specie:	s Data Phas	e TV Activity
Components (3)		+ 13 Fe(s)	FACT53 bee	
		+ 14 Fe(s2)	FACT53 fee	
FeO + ZnO + Fe		10 FeU(s) 16 Fe203(a)	FACT53 Wustite	V
		17 Fe203(s)	FACT53 high-press	sur V
- Products		18 Fe2O3(s3)	FACT53 high-press	sur V
- Contractor - Colution constant	en Calutione	19 Fe3O4(s)	FACT53 magnetite	V
Compound species	om Solutions -	20 Fe304(s2)	FACT53 magnetite	V
gas to local to real 0 - + Base-Phase Full Name 0 in	ked activities	21 Fe3U4(s3) 22 Fe2U4(s4)	FAU153 high-press	sur V
aqueous U I FToxid-SLALiA ASlag-liq D ad	ctivitu coefficir	22 Pesoa(sa)	EACT53 nigripress	ul v
* + pure liquids 1 + FToxid-SPINA ASpinel	Detai	24 ZnO(s)	FACT53 zincite	
* + FToxid-MeO_A AMonoxide	Deta	25 ZnFe204(s)	FACT53 solid	
suppress duplicates apply + FToxid-ZNIT Zincite	dopums	+ 26 Fe2O3(s)	FT oxid hematite	V
* - custom selection		+ 27 Fe2O3(s2)	FT oxid high-press	sur V
species: 7 apply	List	+ 28 Fe2U3(s3)	F I oxid high-press	sur V
	aluda malar u			
	iciude moiar vi			
Legend Legend I Show ⊙ all ⊙ selected IF S	Selecti	ion - Equilit)	
Estimate T(K): 1000 +- selected 3 species: 24 Select 1 Eile	e <u>E</u> dit	Show Sort		
Mass(mol): Select Sele	ected: 1/6 <mark>D</mark>	uplicates selected.	IQUID Sorted I	oy Code
Variables Pha		Species D.	ata Phase	T V Activity
T(C) Zn0/(Fe0+Zn0+ Fe/(Fe0+Zn0+Fe	7 F	ellia) FACTS	53 liquid	
	8 F	eO(lig) FACTS	53 liquid	
	9 5	e304(lin) FACTS	53 liquid	
T(C) vs Zn0/(Fe0+Zn0+Fe)	10 7	official FACTS	53 liquid	
	11 7	n(iiq) FACTS	53 liquid	
FactSage 6.2 beta g:\\PhasFe-Zn-0_Fe0-Zn0-Fe_Fe(S-L),DAT	12 7	nO(liq) FACTO	liquid	
	12 2	no(iiq) n roxic		
Oxide phases				
Stoichiometric metal phases from Fact53	elected	Select All Selec	t/Clear Clear	ОК





FeO - ZnO - Fe



mole Fe/(FeO+ZnO+Fe) = 0.001





FeO-ZnO in Equilibrium with Metals: FSstel vs pure Fe

FeO - ZnO - Fe



mole Fe/(FeO+ZnO+Fe) = 0.001





🕫 Menu - Phase Diagram: FeO-ZnO in equilibriur	m	wi	. 💶 🖂				
<u>Eile U</u> nits <u>P</u> arameters <u>V</u> ariables <u>H</u> elp							
T(C) P(atm) Energy(J) Mass(mol) Vol(litre)		ſ	111 🖳 🕒 🛒				
Components (3)							
FeD + ZnD + Fe	4	🕫 Sele	ection - Eq	uilib		_	
		File E	dit Show Sor	+			
Products				-			
Compound species	l l	Selected: 5	5/17 Duplicates selec	ted. SOLID	Sorted b	y Code	
gas ideal C real 0 * + Base-Phase Full Name		+ Co	de Species	Data	Phase	TV	Activity
aqueous U I Floxid-SLAGA ASiag-liq		+ 13	Fe(s)	FACT53	bee		
t pure solida		14	Fe(s2)	FACT53	fcc		
+ FToxid-Web_A AMONOXide		15	FeO(s)	FACT53	wustite	V	
suppress duplicates apply		16	Fe2O3(s)	FACT53	hematite	V	
species: 5		17	Fe2U3(s2)	FACT53	high-pressure	V	
	1	18	Fe2U3(\$3)	FACT53	high-pressure	V	
	47	19	Fe304(s)	FACT53	magnetite		
Target	1/	20	Fe304(s2)	FACT53	high-pressur	V V	
- none I - immiscible 1 🔽 Show 🖲 all 🔘 selected	4 /	21	Fe304(s3)	FACT53	high-pressur	V	
Estimate T(K): 1000 +- selected 3 species: 24 p 1		23	Zn(s)	EACT53	solid	Y	
Mass(mol): 0 Select		24	$Zn\Omega(s)$	EACT53	zincite		
		25	ZnFe204(s)	FACT53	solid		
Variables	s	+ 26	Fe2O3(s)	FToxid	hematite	V	
T(C) Zn0/(Fe0+Zn0+ Fe/(Fe0+Zn0+Fe		+ 27	Fe2O3(s2)	FToxid	high-pressure	V	
	- /	+ 28	Fe2O3(s3)	FToxid	high-pressure	V	
	1	+ 29	Zn0(s)	FToxid	zincite		
T(C) vs Zn0/(Fe0+Zn0+Fe)							
FactSage 6.2 beta g:\\PhasFe-Zn-0_Fe0-Zn0-Fe_Fe(S-L).DAT			1		1	-	
Oxide phases	ov	v Selected	Select All	Select/Clear	. Clear		OK

Only one metal phase, Fe(s), from Fact53





FeO - ZnO - Fe

mole Fe/(FeO+ZnO+Fe) = 0.001







FeO-ZnO in Equilibrium with Metals: FSstel vs Fe(s)

FeO - ZnO - Fe









FeO-ZnO in Equilibrium with Fe(s) vs FeO-ZnO

FeO - ZnO - Fe

mole Fe/(FeO+ZnO+Fe) = 0.001



2010

wend - mase blagram. Teo-zho in equilibr	u •	Selec	stion - Eq	uilib		_	
Eile <u>U</u> nits <u>P</u> arameters <u>V</u> ariables <u>H</u> elp	Eil	e <u>E</u> di	t Show Sc	ort			
T(C) P(atm) Energy(J) Mass(mol) Vol(litre)	Sel	ected: 7/1	7 Duplicates selec	ted. SOLID	Sorted	by Code	
Components (3)		+ Code	Species	Data	Phase	TV	Activity
FeO + ZnO + Fe	+	13 14	Fe(s) Fe(s2)	FACT53 FACT53	bee fee		
		15	FeO(s)	FACT53	wustite	V	
Products		16	Fe2O3(s)	FACT53	hematite	V	
Compound species Solution species		17	Fe2O3(s2)	FACT53	high-pressur	V	
gas (*) ideal (*		18	Fe2O3(s3)	FACT53	high-pressur	V	
aqueous U I FToxid-SLAGA ASlag-liq		19	Fe304(s)	FACT53	magnetite	V	
+ pure liquids 2 + FT oxid-SPINA ASpinel		20	Fe304(s2)	FACT53	magnetite	V	
* + Proxid-MeU_A AMonoxide		21	Fe304(s3)	FACT53	high-pressur	V	
suppress duplicates apply + FToxid-ZINTI Zincite		22	Fe304(s4)	FACT53	high-pressur	V	
* - custom selection	+	23	∠n(s)	FACT53	solid		
species. 5		24	ZnU(s)	FACT53	zincite		
		25	ZhFeZU4(s)	FAU153	SOlid		
- Target	+	26	Fe2U3(s)	FTOXIC	nematite		
- none -	+	27	Fe203(s2) E-202(s2)	FToxid	high-pressur	V V	
Estimate T(K): 1000 + selected 3	+	20	7e203(83) Ze0(a)	FToxid	nign-pressur	v	
species. 24 Select		23	200(8)	FTOXIC	Zincite	1 1 1	
	(7	Seled	tion - Eq	uilib			
T(C) ZnO/(FeO+ZnO+ Fe/(FeO+ZnO+Fe)	, Ei	e <u>E</u> di	t Show Sc	ort			
	Sel	ected: 2/6	Duplicates selec	ted. LIQUID	Sortec	l by Code]
T(C) vs Zn0/(Fe0+Zn0+Fe)	_ [-	+ Code	Species	Data	Phase	TV	Activity
FactOres C 2 hats	- +	7	Fe(liq)	FACT53	liquid		
Factsage 6.2 beta gt FnasFe-2n-0_Fe0-2n0-Fe_Fe(5-L).DAT		8	FeO(liq)	FACT53	liquid		
Ovida nhasas		9	Fe3O4(liq)	FACT53	liquid		
Oxide pliases	+	10	Zn(liq)	FACT53	liquid		
		11	ZnO(liq)	FACT53	liquid		
Pure Fe and Zn (sol. and liq.) from Fact53	L	12	ZnO(liq)	FToxid	liquid		
Gact Sage [™] Oxides and Py		Selected	Select All	Select/Clear	l Clea	r	ПК

FeO - ZnO - Fe

mole Fe/(FeO+ZnO+Fe) = 0.001







FeO-ZnO in Equilibrium with Fe & Zn (s,l) vs FSstel

FeO - ZnO - Fe

mole Fe/(FeO+ZnO+Fe) = 0.001







– Databases -	3/24 compou	nd databases,	2/22 solution datab	ases ———		
Fact	GactSage"	SGTE	compounds only	Mise	ellane.	ous
 □ ELEM □ FACT ☑ Fact53 ☑ FToxid □ FTsalt □ FTmisc □ FThall □ FThelg □ FTpulp □ FTlite 	 ☐ FScopp ☐ FSlead ☐ FSlite ☑ FSstel ☐ FSupsi ☐ FSnobl Other ☐ OLIP ☐ OLIG 	BINS SGPS SGTE SGnobl SGsold SGnucl TDnucl OLIC OLIL	solutions only no data Clear All Select All Add/Remove Data RefreshDatabases	EXAM	SGSL	□ SGTE*
	<u>O</u> 2 <u>M</u> 0 <u>G</u> 3	<u>kide phas</u> etal phas aseous s	<u>ses</u> ses from FSs species from	<u>tel</u> Fact53		
- Options		ide gaseous ions (p aqueous specie limited data com	lasmas) is ippounds (25C)	imits Irganic species Cx Iinimum solution co	Hy, X(max) = omponents: O	2 1 🖸 2 cpts
Cano	el 🛛		Summary			OK



🕫 Menu - Phase Diagram: FeO-ZnO at metal s	sati 🕫 Selection - Equilib 📃 🗖	×
Eile <u>U</u> nits <u>P</u> arameters <u>V</u> ariables <u>H</u> elp	Eile Edit Show Sort	
T(C) P(atm) Energy(J) Mass(mol) Vol(litre)	Selected: 7/23 Duplicates selected. SOLID Sorted by Code	
Components (3)	+ Code Species Data Phase T V Activity	
FeO + ZnO + Fe	23 Fe304(s2) FACT53 magnetite V 24 Fe304(s3) FACT53 high-pressur V	-
☐ Products	25 Fe3D4(s4) FACT53 high-pressur V	-
Compound species	20 21(s) TACTOS solid 27 ZnD(s) FACT53 zincite	
+ gas i ideal () real 6 × + Base-Phase Full Name ▲ aqueous 0 + ESstel-EE71 EE7N4	▲ 28 ZnFe2D4(s) FACT53 solid	
pure liquids 0 + FSstel-FEZ2 FEZN_DELTA	+ 29 Fe(s) F5stel Dcc_a2 + 30 Fe(s2) F5stel fcc_a1	
* pure solids 7 + FSstel-FEZ3 FEZN_ZETA	31 Fe2O3(s) FSstel hematite V	
suppress duplicates apply + FSstel-HCP HCP_A3:Me2(C,N)	32 Fe304(s) FSstel magnetite V	_
species: 13 + FToxid-SPINA ASpinel	+ 34 Zn(s) F5stel hcp zn o	
+ FToxid-MeD_A AMonoxide	+ 35 Fe2O3(s) FToxid hematite V	
I - Target	→ + 36 Fe2O3(s2) FT oxid high-pressure V	
- none - Legend I - immiscible 1	+ 37 Fe2U3(s3) Floxid high-pressure V + 38 ZnD(s) ET oxid zincite	-
Estimate T(K): 1000 +-selected 12 species: 51 Select		
	Selection - Equilib	\mathbf{X}
Variables	Phi Eile Edit Show Sort	
I(C) ∠nU/(FeU+∠nU+ Fe/(FeU+∠nU+Fe 800 2000 0 1 0.001	Selected: 6/6 GAS Sorted by Code	
	+ Code Species Data Phase T V Activ	rity
	+ 1 0(g) FACT53 gas	
FactSage 6.2 beta g:\\PhasFe-Zn-0_Fe0-Zn0-Fe_FSstel_gas.DAT	+ 2 02(g) FAC105 gas	
Oxide phases, all Metal phases from FSste	e + 4 Fe(g) FACT53 gas	
	+ 5 FeO(g) FACT53 gas	
Gaseous species only from Fact53		_
Gract Sage" Oxides and Py	'YRO ow Selected Select All Select/Clear Clear	ОК



GactSage™

Oxides and Pyrometallurgy 67

CRCT Montreal 2010

FeO - ZnO - Fe





Montreal

2010

Red and blue curves are calculated without gas



FactSage[™]









FeO-ZnO in Equilibrium with Metals at P=100 atm

FeO - ZnO - Fe

P=100 atm, mole Fe/(FeO+ZnO+Fe) = 0.001



GactSage[™]



Fe-Zn-O System








Oxide Phase Diagrams under Reducing Conditions

- Metal phases must be selected
- Step a bit off an oxide section towards metals
- FSstel is needed to see the *right metal phases* in equilibrium
- Metal phases often have only a minor effect on *oxide phase boundaries*
- If you do not have FSstel or SGTE database for metal phases, select metals from Fact53
- Do not forget the gas phase





FeO-CoO System in Equilibrium with Metals

F Components - Phase Diagram	
<u>Eile E</u> dit <u>U</u> nits <u>D</u> ata Search <u>H</u> elp	
T(C) P(atm) Ene	gy(J) Mass(mol) Vol(litre) 👔 📑 📴 🔭
1-3 Con	ponents
FeO CoO	🗷 🖉 Data Search
	-Databases - 3/24 compound databases, 2/22 solution databases
jre j	Cact Cacting" SGTF Miscellaneous
	Compounds only Compounds only Solutions only Solutions only FACT FSLead SGPS no data Fact53 FSlite SGrE Clear All FTsalt FSupsi SGnobl Clear All FThall SGnobl FThall TDnucl Add/Remove Data FTite OLIP OLIC RefreshDatabases
FactSage 6.2 bete Compound: 3/24 databases Solution: Oxide phases, Gaseous spe Metal phases from ESstel	Vext >> 2/22 databases Default Include (nlasmas) Imited data compounds (25C) Cancel Summary
Gact Sage [™]	Oxides and Pyrometallurgy 74 CRCT Montreal 2010

FeO-CoO System in Equilibrium with Metals

F Menu - Phase Diagra	am: FeO-CoO-Fe	at metal satura	tion using 🔳 🗆 🔀			
Eile <u>U</u> nits <u>P</u> arameters <u>V</u> ariab	oles <u>H</u> elp					
🗅 😂 🖬 T(C) P(atm) Energy(J) Mass(mol) Vol(litre) 🏢 🖳 🐺						
Components (3)						
	FeO + Co	oO + Fe				
Products						
Compound species	-Solution species		Custom Solutions			
+ gas (© ideal () real 6	+ Base-Phase	Full Name	0 fixed activities 0 ideal solutions			
aqueous U	+ FSstel-FCC	FCC_A1:Me(C,N)	0 activity coefficients			
pure liquids U	+ FSstel-BCC	BUU_A2	Details			
+ pure solids	+ FSstel-FE-L					
suppress duplicates apply		ASleg-lig	- Pseudonyms			
custom selection species: 17	+ EToxid-SPINA	ASpinel	apply 🔽 List			
	I FToxid-MeO_A	AMonoxide				
			I include molar volumes			
- Target	_Legend		Total Species (max 1500) 58			
- none -	I-immiscible 2	Show 🖲 all 🔿 selected	Total Solutions (max 40) 9			
Estimate T(K): 1000	+-selected 5	species: 41				
Mass(mol):		solutions: 9 Select	Default			
Variables			Phase Diagram			
T(C) CoO/(FeO+CoO)	T(C) CoO/(FeO+CoO) Fe/(FeO+CoO)					
100 1300 0 1	0.001		' <u>L</u>			
			Calculate >>			
FactSage 6.2 beta C:\\Phas	:Co-Fe-O_FeO-CoO-Fe_FSstel.E	TAC				











FeO-CoO System in Equilibrium with Metals

FeO - CoO - Fe

mole Fe/(FeO+CoO) = 0.001



2010

FeO-CoO System in Equilibrium with Pure Fe and Co

Gact	- Z724 Compoun			i Mie	collano	nus
 □ ELEM □ FACT ☑ Fact53 ☑ FToxid □ FTsalt □ FTmisc 	FScopp FSlead FSlite FSstel FSupsi FSnobl	BINS BINS SGPS SGTE SGnobl SGsold SGnucl	Compounds only solutions only no data Clear All Select All			SGTE
FThall FThelg FTpulp FTlite Including aquiv	Other	TDnucl	Add/Remove Data RefreshDatabases aqueous (hydrometallur	gical) calculation	s at or near room	n temperature.
daseous ions	(plasmas)		nt in including the aqueo	ous species. This	option has no e	ffect upon
- Options	i(plasmas).	ide gaseous ions (nlasmas) aqueous specie	nt in including the aqueo	ous species. This es, Gase es from F Limits Drganic species C	option has no e OUS SPEC act53 XHy, X(max) =	ffect upon



FeO-CoO System in Equilibrium with Pure Fe and Co

F Menu - Phase Diagram: comments		
File Units Parameters Variables Help		
T(C) P(atm) Energy(J) Mass(mol) Vol(litre)	11 🕒 🕒 🐨	
Components (3)		
FeO + CoO + Fe		
Products	🕞 Selection - Equilib	
Compound species Solution species	Eile Edit Show Sort	
+ gas (ideal real * + Base-Phase Full Name aqueous 0 1 FToxid-SLAGA ASlag-liq	Selected: 8/19 Duplicates selected. SOLID Sorted by Code	
pure liquids 0 + FToxid-SPINA ASpinel	+ Code Species Data Phase TV Activ	/itv
+ Floxid-MeU_A AMonoxide	+ 13 Fe(s) FACT53 bcc	
suppress duplicates apply	F + 14 Fe(s2) FACT53 fcc	
*- custom selection	15 FeO(s) FACT53 wustite V	
species: 12	16 Fe2O3(s) FACT53 hematite V	
	Fe2O3(s2) FACT53 high-pressur V	
	- 18 Fe2O3(s3) FACT53 high-pressur V	
Legend Key G all C salasted	19 Fe3O4(s) FACT53 magnetite V	
I-immiscible 1	20 Fe3O4(s2) FACT53 magnetite V	
Estimate T(K): 1000 +-selected 2 species: 29	21 Fe3O4(s3) FACT53 high-pressur V	
Mass(mol): 0 solutions: 4	22 Fe3O4(s4) FACT53 high-pressur V	
	+ 23 Co(s) FACT53 solid	
_Variables	Phas + 24 Co(s2) FACT53 solid	
	25 CoO(s) FACT53 solid	
(G) GSG/(GS-GSG) 10/(GS-GSG) Y	26 Co3O4(s) FACT53 solid	
	X 27 (CoO)(Fe2O3)(s) FACT53 solid o	
	+ <mark>28</mark> Fe2O3(s) FToxid hematite V	
	+ <mark>29</mark> Fe2O3(s2) FToxid high-pressur V	
	+ <mark>30 </mark> Fe2O3(s3) FToxid high-pressur V	
FactSage 6.2 heta C1 \PhasCo-Fe-0, Fe0-Co0-Fe, Pure-Co DAT	+ <mark>31 C</mark> oO(s) FToxid solid	
<u>Oxide phases</u>		
<u>Fe and Co from Fact53</u>	pw Selected Select All Select/Clear Clear	0К





FeO-CoO System in Equilibrium with Pure Fe and Co

FeO - CoO - Fe

mole Fe/(FeO+CoO) = 0.001



FeO-CoO in Equilibrium with Fe and Co vs FSstel

FeO - CoO - Co

mole Co/(FeO+CoO) = 0.001



FeO-CoO System in Equilibrium with Pure Co

FeO - CoO - Fe *mole Fe/(FeO+CoO) = 0.001* 1300 1100 AMonoxide + Co(s2)900 T(C) 700 ASpinel + Co(s2)500 300 ASpinel + Co(s)100 0.2 0.4 0.6 0.8 0 1 mole CoO/(FeO+CoO)





FeO-CoO System in Equilibrium with Pure Fe





FactSage[™]



Fe-Co-O System in Equilibrium with Metals

F Menu - Phase Diagra	am: Using FSstel for metallic phases 🛛 📃 🗖 🔀				
Eile Units Parameters Variables Help T(C) P(atm) Energy(J) Mass(mol) Vol(litre) Components (3) Fe + Co + 0					
Products Compound species * + gas • ideal C real 1 aqueous 0 pure liquids 0 * + pure solids 4 suppress duplicates apply *- custom selection species: 5	Solution species * Base-Phase Full Name + FSstel-FCC FCC_A1:Me(C,N) + FSstel-BCC BCC_A2 + FSstel-FE-L Fe-LIQUID + FSstel-HCP HCP_A3:Me2(C,N) 1 FToxid-SLAGA ASlag-liq + FToxid-SPINA ASpinel + FToxid-MeO_A AMonoxide				
- Target - none - Estimate T(K): 1000 Mass(mol): 0	Legend I-immiscible 1 +-selected 6 Species: 38 solutions: 8 Select Default Default				
Variables T(C) O/(Fe+Co+O) 700 0 1	Co/(Fe+Co+O)				
A = 0, B = Fe, C = Co	B C C Calculate >>				
FactSage 6.2 beta C:\CAD\	\All Diagrams\PhasCo-Fe-O_700C_FSstel.DAT				





Fe-Co-O System in Equilibrium with Metals

Variables Y C C X A B C Y steps: 5 X steps: 5	ompositions 2 og10(a) 💌 0 Next >>	Temperat	ture constant 700	Pressure Pressure P(atm)	istant
#1. 1 Fe	(mole) + 0 Co + + 1 Co +	10 10	A-Corner 1 (max) 0 (min)		
#2 . 0 Fe	+ 1 Co + + 1 Co +	0 0 1 0	C-Corner 1 (max) 0 (min)		
#3. 1 Fe	+ 0 Co + + 1 Co +	0 0 1 0	B-Corner 1 (max) 0 (min)		
		Cancel			ОК





Fe-Co-O System in Equilibrium with Metals



Fe-Co-O System in Equilibrium with Pure Metals

👎 Menu - Phase Diagram: last system	
Eile <u>U</u> nits <u>P</u> arameters <u>V</u> ariables <u>H</u> elp	
🗅 🕼 🖬 T(C) P(atm) Energy(J) Mass(mol) Vol(litre)	
	E Selection - Equilib
Components (3)	
Fe + Co + O	Eile Edit Show Sort
	Selected: 8/19 Duplicates selected. SOLID Sorted by Code
- Products	
Compound species	+ Code Species Data Phase T V Activity
Figas • ideal Circal 6	+ 13 Fe(s) FACT53 bcc
aqueous 0 I FToxid-SLAGA ASlag-lig	+ 14 $Fe(sz)$ FAC153 TCC 15 $FeO(c)$ EACT53 wulletite V
* F pure liquids 2 + FToxid-SPINA ASpinel	16 Fe2O3(s) FACT53 weisite V
* + pure solids 8 + FToxid-MeO_A AMonoxide	17 Fe2O3(s2) FACT53 high-pressur V
suppress duplicates apply	18 Fe2O3(s3) FACT53 high-pressur V
*- custom selection	19 Fe3O4(s) FACT53 magnetite V
species: 16	20 Fe3O4(s2) FACT53 magnetite V
	21 Fe3O4(s3) FACT53 high-pressur V
	22 Fe3O4(s4) FACT53 high-pressur V
-Target	+ 23 Co(s) FACT53 solid
-none -	+ 24 Co(s2) FACT53 solid
Estimate T(K): 1000 +-selected 2 aposios: 20	25 CoO(s) FACT53 solid
species. 23 Select	26 Co3O4(s) FACT53 solid
Mass(mol):	27 (CoO)(Fe2O3)(s) FACT53 solid o
	+ <mark>28 </mark> Fe2O3(s) FToxid hematite V
Pha	³ + <mark>29 </mark> Fe2O3(s2) FToxid high-pressur V
T(C) 0/(Fe+Co+0) Co/(Fe+Co+0) A	+ 30 Fe2O3(s3) FToxid high-pressur V
700 01 01	+ 31 CoO(s) FToxid solid
рани и правити и	1
A = 0, B = Fe, C = Co	
FertSero 6.2 hote	pw Selected Select All Select/Clear Clear OK
r actorye ole beta	

Oxide phases

Fe and Co from Fact53





Fe-Co-O System in Equilibrium with Pure Metals



Fe₂O₃-Cr₂O₃ System in Equilibrium with Air

F Menu - Phase Diagram: Fe2O3-Cr2O3-O2 at P(O2)=0.21	1 atm 📃 🗖 🔀
<u>Eile U</u> nits <u>P</u> arameters <u>V</u> ariables <u>H</u> elp	
T(C) P(atm) Energy(J) Mass(mol) Vol(litre)	111 🖳 🖳 🐨
Components (3)	E Selection - Equilib
Fe2O3 + Cr2O3 + O2	Eile Edit Show Sort
	Selected: 4/23 Dunlicetes, selected SOLID Sorted by Code
Products	
Compound species Solution species	+ Code Species Data Phase T V Activity
+ gas (ideal C real 9 * + Base-Phase Full Name	19 Cr(s) FACT53 solid
aqueous 0 I FToxid-SLAGA ASlag-liq	20 CrO2(s) FACT53 solid o
pure liquids 0 + FToxid-SPINA ASpinel	21 CrO3(s) FACT53 solid
* FToxid-MeO_A AMonoxide	22 Cr2O3(s) FACT53 solid
suppress duplicates apply + FToxid-CORU M2O3(Corundum)	c 23 Cr3O4(s) FACT53 solid o
*- custom selection	24 Cr5012(s) FACT53 solid o
species: 13	25 Cr8O21(s) FACT53 solid o
	A 26 Fe(s) FACT53 bcc
	27 Fe(s2) FACT53 fcc
Target	28 FeO(s) FACT53 wustite V
- none - I-immiscible 1 🗹 Show 🖲 all 🔘 selected 🛛	T Fe2O3(s) FACT53 hematite V
Estimate T(K): 1000 +-selected 3 species: 29	30 Fe2O3(s2) FACT53 high-pressur V
Mass(mal)	31 Fe2O3(s3) FACT53 high-pressur V
	32 Fe3O4(s) FACT53 magnetite V
	- 33 Fe3O4(s2) FACT53 magnetite V
Variables Phas	IS 34 Fe3O4(s3) FAC153 high-pressur V
1 (C) log10(p(02)) Cr2O3/(Fe2O3+Cr	35 Fe3O4(s4) FACT53 high-pressur V
1300 2500 -0.67778 01	36 FeCr2O4(s) FAC153 solid
	+ 37 Cr2U3(s) Filoxid solid
T(C) vs Cr203/(Fe203+Cr203)	38 Cr304(s) Filoxid solid o
	+ 30 Fe2O3(s) Filoxid hematite V
	+ 40 Fe2O3(sz) Filoxia high-pressur V
HactSage 6.2 beta U:\\PhasUt-Fe-U_Fe2U3-Ct2U3-U2_P(U2).DAT	je nerovice nign-pressur V
<u>Gas phase must be selected</u> even though it does not form	ow Selected Select All Select/Clear Clear OK





Fe₂O₃-Cr₂O₃ System in Equilibrium with Air

F Variables: Fe2O3-Cr2O3-O2 T(C) vs composition #1.







Fe₂O₃-Cr₂O₃ System in Equilibrium with Air

 $Fe_2O_3 - Cr_2O_3 - O_2$ $p(O_2) = 0.21 atm$



y <u>U</u> nits <u>P</u> arameters <u>V</u> ariables <u>H</u> elp	₽ Se	elect	ion - Equili	Ь			
T(C) P(atm) Energy(J) Mass(mol) Vol(litre)	Eile	<u>E</u> dit	Show Sort				
omponents (3)	Selec	ted: 2/13	Duplicates select	ted. SOLID	Sorted	by Code	
MgO + Cr2O3 + O2	+	Code	Species	Data	Phase	TV	Activity
		20	Mg(s)	FACT53	solid		
roducts		21	MgO(s)	FACT53	periclase		
Compound species		22	Cr(s)	FACT53	solid		
F gas • ideal • real 10 * + Base-Phase Full Name		23	CrO2(s)	FACT53	solid	0	
		24	CrO3(s)	FACT53	solid		
pure liquids 0 + FToxid-SPINA ASpinel		25	Cr2O3(s)	FACT53	solid		
pure solids 2 t EToxid-MeD A AMonovide		26	Cr3O4(s)	FACT53	solid	0	
		27	Cr5012(s)	FACT53	solid	0	
I suppress duplicates apply		28	Cr8O21(s)	FACT53	solid	0	
- custom selection		29	(MgO)(Cr2O3)(s)	FACT53	chromite		
species. 12	+	30	MgO(s)	FToxid	periclase	V	
]+	31	.Cr2O3(s)	Elloxid	solid		
TargetLegend Legend Show ● all ● selected	F Se	elect	ion - Equili	b			
Target Legend • none - I - immiscible 1 Estimate T(K): 1000 Mass(mol): 0	F Se Eile Selec	elect Edit ted: 10/1	ion - Equili Show Sort 0	GAS	Sorted by	Code	
Target - none - Estimate T(K): 1000 Mass(mol): 0 Ariables Masset (mol): 0 Masset (mol): 0 Ariables Masset (mol): 0 Ariables Masset (mol): 0 Ariables Aria	F Selec	Edit Edit ted: 10/1	ion - Equili Show Sort 0 Species	GAS Data	Sorted by	Code	Activit
Target Legend - none - I - immiscible 1 Estimate T(K): 1000 Mass(mol): Immiscible 2 Mass(mol): Immiscible 2 ariables Pha T(C) log10(p(O2))	F Select	Edit Edit ted: 10/1 Code	ion - Equili Show Sort 0 Species	GAS GAS Data FACT53	Sorted by 1 Phase gas	Code	Activit
Target Legend -none - I - immiscible 1 Estimate T(K): 1000 Mass(mol): Immiscible 2 Mass(mol): Immiscible 2 ariables Pha T(C) log10(p(O2)) Cr2O3/(MgO+Cr2 Y	F So Eile Selec	Edit Edit ted: 10/1 Code	ion - Equili Show Sort 0 0 (g) 02(g)	GAS GAS FACT53 FACT53	Sorted by I Phase gas gas		Activit
Target Legend Image: Legend <t< td=""><td>F Selec</td><td>Edit Edit ted: 10/1 Code 1 2 3</td><td>ion - Equili Show Sort 0 0 (g) 02(g) 03(g)</td><td>GAS GAS FACT53 FACT53 FACT53</td><td>Sorted by I Phase gas gas gas</td><td>Code</td><td>Activit</td></t<>	F Selec	Edit Edit ted: 10/1 Code 1 2 3	ion - Equili Show Sort 0 0 (g) 02(g) 03(g)	GAS GAS FACT53 FACT53 FACT53	Sorted by I Phase gas gas gas	Code	Activit
Target Legend - none - - Estimate T(K): 1000 Mass(mol): Image: Selected 2 Mass(mol): Image: Selected 2 ariables T(C) 1000 3000 -5.5 01 Image: Selected 2 (C) vs Cr203/(Mg0+Cr203)	F Select a + + + + + +	Edit Edit Code 1 2 3 4	ion - Equili Show Sort 0 Species 0(g) 02(g) 03(g) Mg(g)	GAS GAS FACT53 FACT53 FACT53 FACT53 FACT53	Sorted by Phase gas gas gas gas gas	Code	Activit
Target Legend Image: Species: 17 Select Image: Species: 17 Select Select Image: Species: 17 Select	F Select a + + + + + + +	Edit Edit Code 1 2 3 4 5	ion - Equili Show Sort 0 0 0(g) 02(g) 03(g) Mg(g) Mg2(g)	GAS GAS FACT53 FACT53 FACT53 FACT53 FACT53 FACT53	Sorted by Phase gas gas gas gas gas gas	Code	Activit
Target Legend -none - I-immiscible 1 Estimate T(K): 1000 Mass(mol): Selected 2 ariables solutions: T(C) log10(p(02)) Cr203/(MgO+Cr2 Y 1000 3000 -5.5 01 (C) vs Cr203/(MgO+Cr203)	F Select Eile Select + + + + + + +	Edit Edit Code 1 2 3 4 5 6	ion - Equili Show Sort 0 0 0(g) 02(g) 03(g) Mg(g) Mg2(g) Mg2(g)	GAS GAS FACT53 FACT53 FACT53 FACT53 FACT53 FACT53 FACT53 FACT53	Sorted by C Phase gas gas gas gas gas gas gas gas		Activit
Target Legend Image: Constraint of the selected - none - Image: Constraint of the selected Image: Constraint of the selected Estimate T(K): 1000 Select Select Mass(mol): Image: Constraint of the selected Select Select ariables Image: Constraint of the selected Image: Constraint of the selected Phate 1000 3000 -5.5 0.1 Image: Constraint of the selected of the selected Image: Constraint of the selected o	F Select Eile Select + + + + + + + + +	Edit Edit Code 1 2 3 4 5 6 7	ion - Equili Show Sort 0 0 0(g) 02(g) 03(g) Mg(g) Mg2(g) Mg2(g) Mg2(g) Cr(g)	GAS GAS FACT53 FACT53 FACT53 FACT53 FACT53 FACT53 FACT53 FACT53 FACT53	Sorted by I Phase gas gas gas gas gas gas gas gas		Activit
Target Legend Image: Show ● all ● selected - none - Image: Show ● all ● selected species: 17 Estimate T(K): 1000 solutions: 4 select Mass(mol): Image: Selected 2 solutions: 4 select ariables T(C) log10(p(O2)) Cr2O3/(MgO+Cr2 Pha 1000 3000 -5.5 0.1 Image: Selected 2 Y (C) vs Cr2O3/(MgO+Cr2O3) C:\\PhasCr-Mg-0_MgO-Cr2O3-O2_P(O2).DAT Selected 2	F Selec Eile Selec + + + + + + + + + + +	Edit Edit Code 1 2 3 4 5 6 7 8 8	ion - Equili Show Sort 0 0 0(g) 02(g) 03(g) Mg(g) Mg2(g) Mg2(g) Mg0(g) Cr(g) Cr(g)	GAS GAS FACT53 FACT53	Sorted by I Sorted by I gas gas gas gas gas gas gas gas		Activit
Farget Legend ✓ Show ● all ● selected Estimate T(K): 1000 species: 17 Mass(mol): Select solutions: 4 ariables T(C) log10(p(02)) Cr2O3/(MgO+Cr2 Pha 1000 3000 -5.5 0.1 ✓ ✓ (C) vs Cr2O3/(MgO+Cr2O3) C:\\PhasCr-Mg-O_MgO-Cr2O3-O2_P(02).DAT ✓	F Selec Eile Selec 4 + + + + + + + + + + + +	Edit Edit ted: 10/1 Code 1 2 3 4 5 6 7 8 9 10	ion - Equili Show Sort 0 0 0(g) 02(g) 03(g) Mg(g) Mg2(g) Mg2(g) Mg2(g) Mg0(g) Cr(g) Cr0(g) Cr02(g) Cr02(g)	GAS GAS FACT53 FACT53	Sorted by Control by C		Activit
Target Legend ✓ Show ● all ● selected Estimate T(K): 1000 species: 17 Mass(mol): 0 Select species: 17 ariables T(C) log10(p(O2)) Cr2O3/(MgO+Cr2 Pha 1000 3000 -5.5 0.1 ✓ ✓ (C) vs Cr2O3/(MgO+Cr2O3) C:\\PhasCr-Mg-O_MgO-Cr2O3-O2_P(O2).DAT ✓	F Select File Select * * * * * * * * * * * *	Edit Edit Code 1 2 3 4 5 6 7 8 9 9 10	ion - Equili Show Sort 0 0(g) 02(g) 03(g) 03(g) Mg0(g) Mg0(g) Mg0(g) Cr(g) Cr0(g) Cr02(g) Cr02(g) Cr03(a)	GAS GAS FACT53	Sorted by I Sorted by I gas gas gas gas gas gas gas gas	Code TV	Activit

F Variables: MgO-Cr2	203-02 T(C) vs composition #1. 🛛 🔀
Variables compositions 1 Y ● compositions 1 A log10(a) 1 B C V 1 Y steps: 5 Next >>	Temperature Y-axis T(C) Y-axis Max: 3000 1/TK Max: Min: 1000
Chemical Potentials #1. log10(p) = constant ▼ O2 ▼ gas-FACT53 ▼ -5.5	Compositions (mole) #1. 0 MgO + 1 Cr2O3 X-axis 1 MgO + 1 Cr2O3 1 (max) 0 (min) 0 (min)
	Cancel OK





 $MgO - Cr_2O_3 - O_2$ $p(O_2) = 10^{5.5} atm$



2010

F Menu - Phase Diagram: comments	
<u>Eile U</u> nits <u>P</u> arameters <u>V</u> ariables <u>H</u> elp	
T(C) P(atm) Energy(J) Mass(mol) Vol(litre)	11 🕒 🕒
Components (3) MgO + Cr2O3 + O2	
Products	
Compound species Solution species * + gas (• ideal (• real 10) * + Base-Phase Full Name aqueous 0 I FToxid-SLAGA ASlag-liq	F Selection - Equilib
pure liquids 0 + FToxid-SPINA ASpinel * + pure solids 2 + FToxid-MeO_A AMonoxide	Selected: 10/10 GAS Sorted by Code
*- custom selection species: 12	+ Code Species Data Phase T V Activity ! 1 O(g) FACT53 gas Image: Compare the second sec
	! 3 O3(q) FACT53 gas
Target	I 4 Mg(g) FACT53 gas
-none - I-immiscible 1 I Show ● all ● selected	- ! 5 Mg2(g) FACT53 gas
Estimate T(K): 1000 +-selected 2 species: 17	I 6 MgU(g) FAC153 gas
Mass(mol): 0 solutions: 4	PAC153 gas
	I 9 CrO2(g) FACT53 gas
	Phas I 10 CrO3(g) FACT53 gas
T(C) logTU(p(U2)) C/2U3/(MgU+C/2	Y
1000 3000 -5.5 0 1	×
T(C) vs Cr2O3/(MgO+Cr2O3)	ow Selected Select All Select/Clear Clear OK
FactSage 6.2 beta C:\\PhasCr-Mg-0_Mg0-Cr2O3-O2_P(O2)_gas-metastable.DAT	

Gas phase must be selected,

but it can be made dormant





 $MgO - Cr_2O_3 - O_2$ $p(O_2) = 10^{5.5} atm$



Fe-Cr-O System at 1300 ℃

F Components - Phase Dia	agram	
File Edit Units Data Search Help		
	T(C) P(atm) Energy(J) Mass(mol) Vol(litre)) III 🔛 🗁 🗠 🖓
1-3		🕼 Data Search 🛛 🔀
		– Databases - 3/24 compound databases, 2/22 solution databases —
	Componente	Compounds only Miscellaneous
	Fe	ELEM FScopp BINS SGSL SGTE* SGSL SGTE*
		Fact53 FSlite SGTE
	[여 	FTsalt SGood SGood
	02	FTmisc FSnobl SGnucl Select All
		FThelg Other Doucl Add/Remove Data
		FTlite OLIG OLIL RefreshDatabases
		Information -
		Oxide phases
		Metal phases from FSstel
		- Options
		Default gaseous ions Organic species CxHy, X(max) = 2
		✓ Imited data compounds (25C)
		Cancel Summary OK
	Next >>	
FactSage 6.2 beta Compound: 3/24 databas	es Solution: 2/22 databases	





Fe-Cr-O System at 1300 ℃

F Menu - Phase Diagram: last system			
<u>Eile U</u> nits <u>P</u> arameters <u>V</u> ariables <u>H</u> elp			
□ 🛎 🖬 T(C) P(atm) Energy(J) Mass(mol) Vol(litre)			
Components (3) Fe + Cr + O2			
Products	E Soloction Equilib		
Compound species Solution species Solution species			
gas 💿 ideal 🔿 real 0 🔹 + Base-Phase Full Name	<u>E</u> ile <u>E</u> dit Show Sort		
aqueous 0 + FSstel-FCC FCC_A1:Me(C,N)			
pure liquids 0 + FSstel-BCC BCC_A2	Selected: 5/31 Duplicates selected. SOLID Sorted by Code		
★ pure solids 5 ★ FSstel-SIGM SIGMA	+ Code Species Data Phase T.V. Activity		
suppress duplicates apply + FSstel-FE-L Fe-LIQUID	-F 36 Fe304(s) FACT53 magnetite V		
*- custom selection I FToxid-SLAGA ASlag-liq	37 Fe304(s2) FACT53 magnetite V		
species: 5 + FToxid-SPINA ASpinel	38 Fe3O4(s3) FACT53 high-pressur V		
+ FToxid-MeO_A AMonoxide	Fe3O4(s4) FACT53 high-pressur V		
+ FToxid-CORU M2O3(Corundum)	40 FeCr2O4(s) FACT53 solid		
- Target	41 Cr(s) FSstel bcc_a2		
-none- I-immiscible 1 I Show (● all () selected	- 42 Cr2O3(s) FSstel solid		
Estimate T(K): 1000 +-selected 7 species: 40 Select	43 Fe(s) FSstel bcc_a2		
Mass(mol): 0	44 Fe(s2) FSstel fcc_a1		
	45 Fe2O3(s) FSstel hematite V		
- Variables	15 Fe3O4(s) FSstel magnetite V		
T(C) log10(p(O2)) Cr/(Ee+Cr)	47 Fe3O4(s2) FSstel magnetite V		
Y	48 FeCr2O4(s) FSstel solid		
	× + <mark>49 C</mark> r2O3(s) FToxid solid		
$\left[\log(10(n(O2))) (\text{stm}) + n Cr/(E_{O+}C)\right]$	+ <mark>50 C</mark> r3O4(s) FToxid solid o		
	+ <mark>51 F</mark> e2O3(s) FToxid hematite V		
	+ <mark>52 F</mark> e2O3(s2) FToxid high-pressur V		
FactSage 6.2 beta C:\\PhasCr-Fe-0 1300C Variable-P(02).DAT	─ + <mark>53 F</mark> e2O3(s3) FToxid hiqh-pressur V		
<u>Oxide phases</u>			
	ow Selected Select All Select/Clear Clear OK		
Nothing from Fact53 and from FSstel			





Fe-Cr-O System at 1300 ℃

F Variables: Fe-Cr-O2 log10(p(O2)) (atm) vs compositio...

Variables Y X A C B C Y steps: 5 X steps: 5	compositions 1 log10(a) 1 Next >>	 Temperature T(C) T(C) I300 Pressure P(atm) Constant Iog P I
Chemical Potentials #1. log10(p) = Y-axis O2 0 gas-FACT53 -20 Compositions (mole) #1. 0 Fe + 1 0 (min)		
		Cancel OK





