

Oxides and Pyrometallurgy

- **Copper Extraction from Sulfide Concentrates**

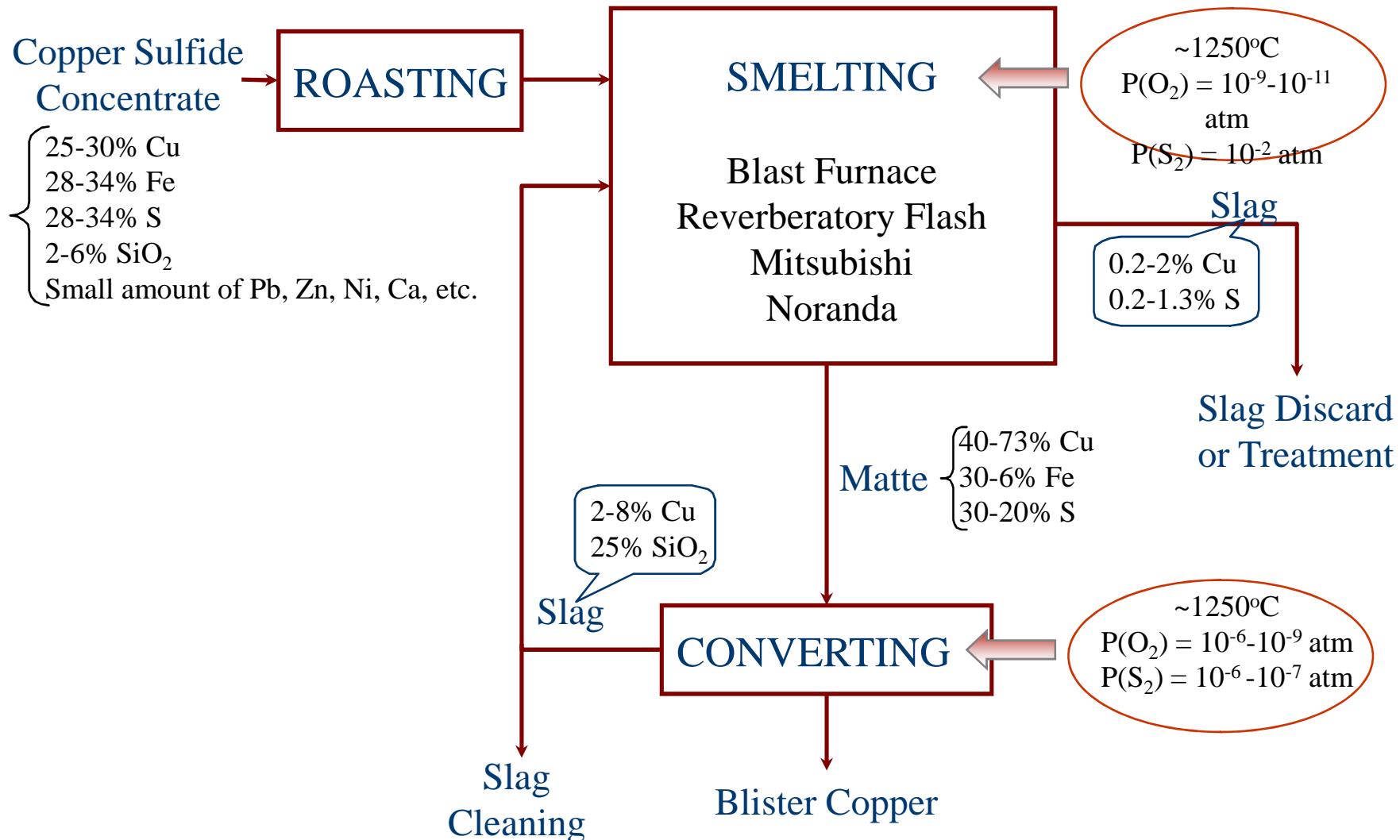
- **Using Equilib Program**

- 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

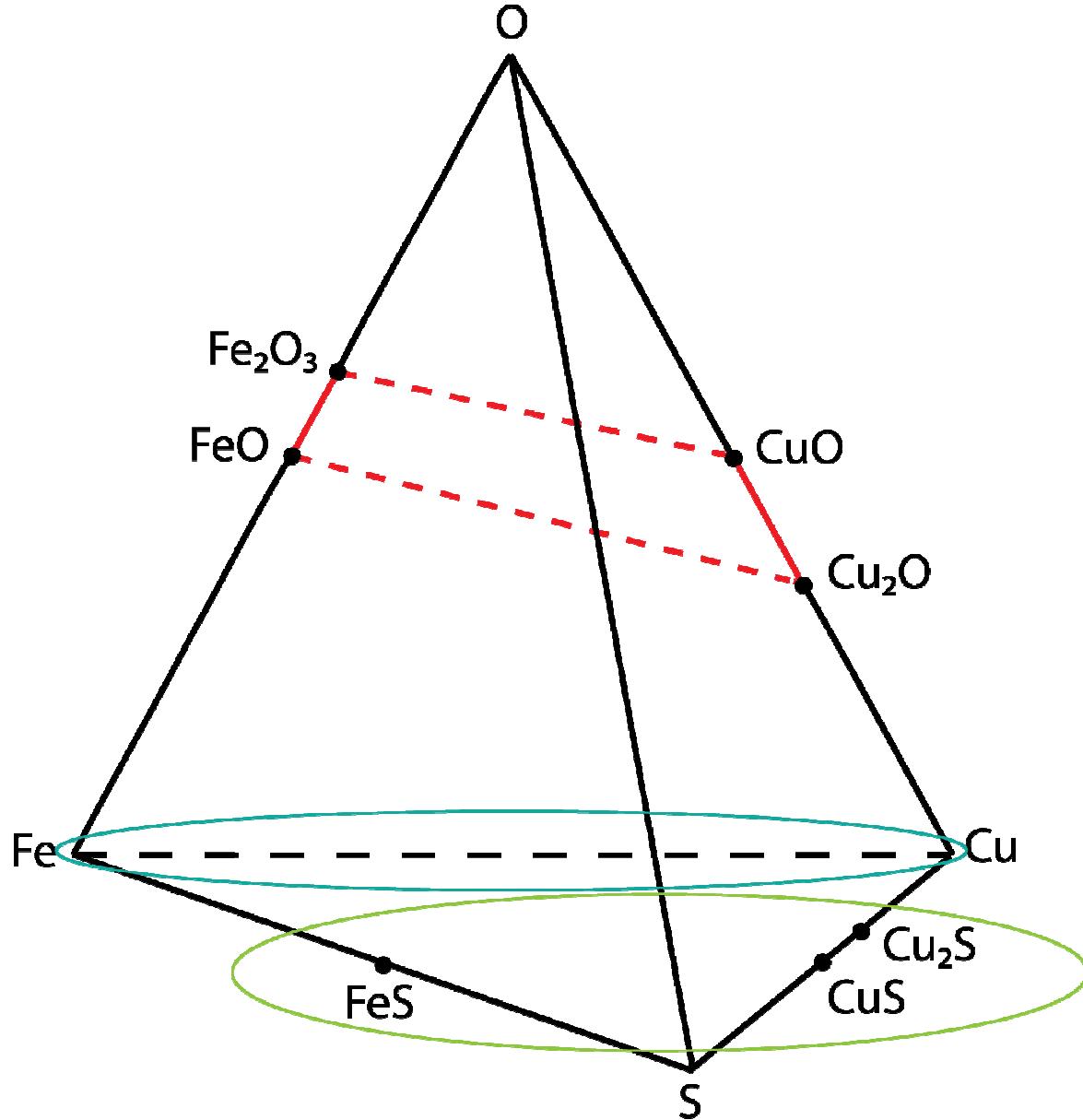
Copper Extraction from Sulfide Concentrates



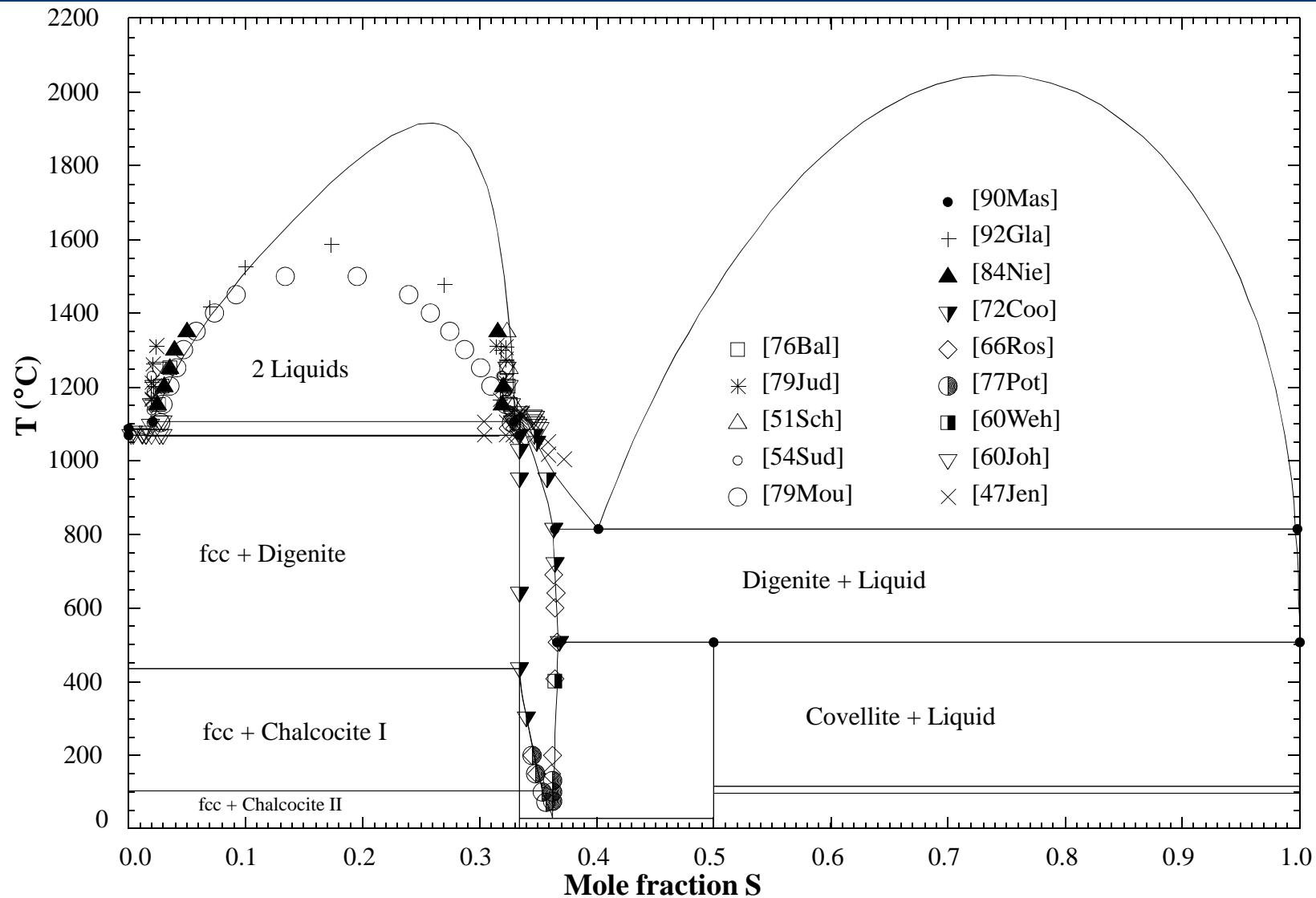
Direct Smelting: Matte/Slag/Cu equilibrium

- 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(O₂), vary Fe/SiO₂
 - 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

Fe-Cu-O-S System



Cu-S System



Selection of Databases

FactSage 6.1 - Summary of Databases

Overview of databases

Compound Databases :

FACT53 - FACT 5.3 compound database:

SGPS - SGTE pure substances database

Gaseous species

Coupled Compound & Solution Databases :



Package:

FToxid - oxide database for slags, glasses, ceramics, refractories

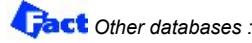
FTsalt - salt database

FThall - Hall aluminum database

FTheig - aqueous (Helgeson) database

FTmisc - miscellaneous database for sulfides, alloys, etc.

FTpulp - pulp and paper database (and corrosion and combustion)



Other databases :

FTlite - light metal database (formerly FSlite)

Slag, Oxides

Matte, Sulfides, Liquid metals

Metal phases



Databases:

V FSropp - copper alloy database

V FSlead - lead alloy database

FSstel - steel database

FSupsi - ultrapure silicon database

Metal phases



Databases:

V SGnobl - noble metal database (formerly FSnobl)

SGnucl - nuclear database

SGTE(2007) - alloy database (formerly SGTE (2004))

V SGsold - solders database

BINARY - (2004) free alloy database

Other Databases:

TDNucl - Thermodata nuclear database

Metal phases

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

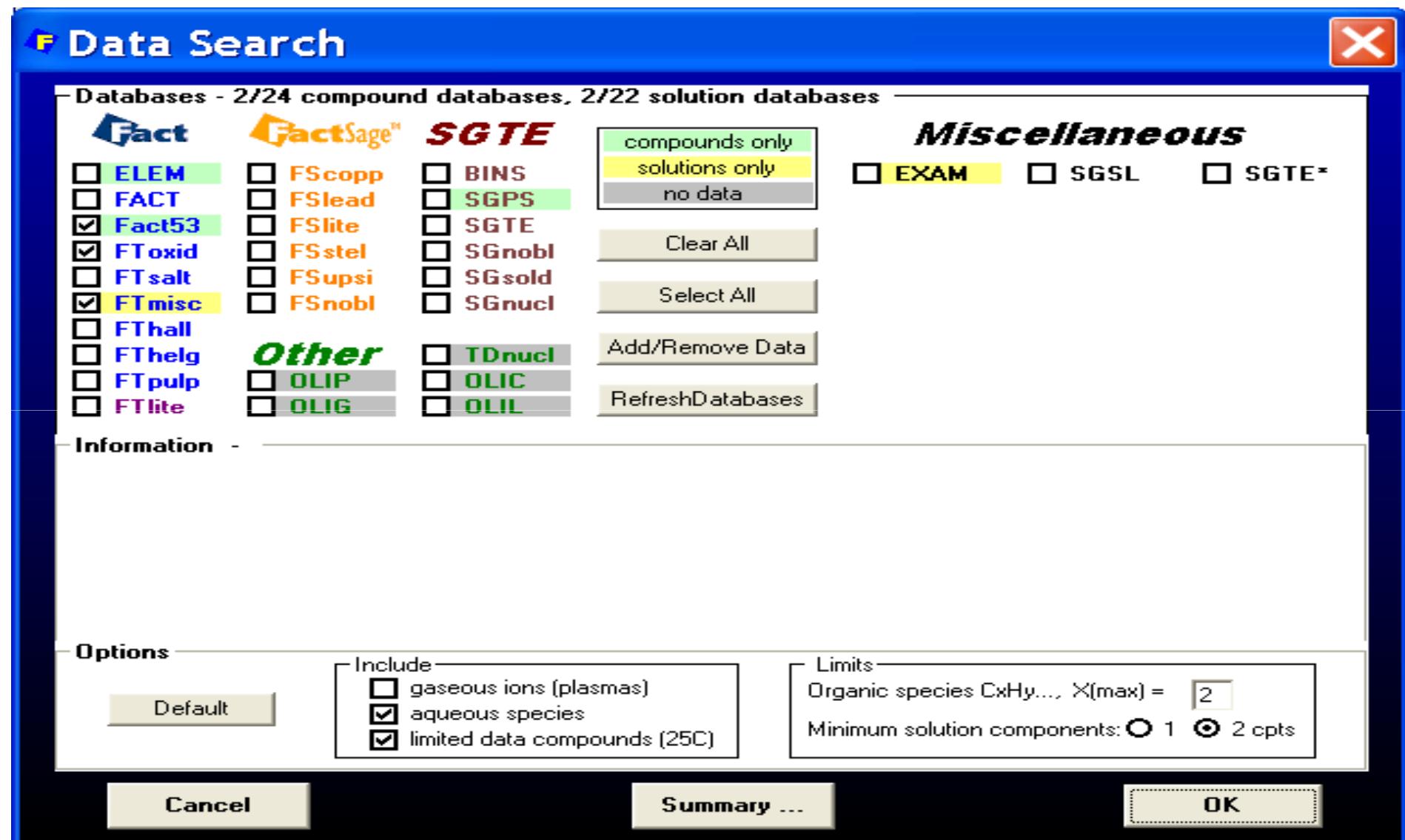
It is not consistent with solid sulfide phases

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

- Liquid Fe [FTmisc-FeLQ] with dilute solutes **Al, 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 solutes **Ag, As, Au, Bi, Cu, Fe, Na, O, S, Sb, Sn, Zn**

Selection of Databases



Input for Having Matte + Slag + Cu in Equilibrium

Reactants - Equilib

File Edit Table Units Data Search Help

T(C) P(atm) Energy(J) Mass(g) Vol(litre)

1 - 7

Mass(g)	Species	Phase	T(C)	P(total)**	Stream#	Data
100	Cu ₂ S				1	
+ 100	Cu				1	
+ <A>	FeO				1	
+ <100-A>	SiO ₂				1	
+ 0	CaO				1	
+ 0.001	Pb				1	
+ 0.001	Zn				1	

Initial Conditions

Next >>

FactSage 6.2 bet. Compound: 2/24 databases Solution: 2/22 databases

Fixing Oxygen Pressure

Selection - Equilib T(C) = 1250...

File Edit Show Sort

Selected: 38/38 GAS Sorte Page 20 Refresh

	Code	Species	Data	Phase	T	V	Activity
+	1	O(g)	FACT5	gas			5.4928E-10
+a	2	O2(g)	FACT5	gas			
+	3	O3(g)	FACT5	gas			3.3595E-21
+	4	Si(g)	FACT5	gas			7.0399E-23
+	5	Si2(g)	FACT5	gas			4.1834E-40
+	6	Si3(g)	FACT5	gas			3.1255E-55
+	7	SiO(g)	FACT5	gas			2.8338E-11
+	8	S(g)	FACT5	gas			7.4003E-08
+	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 Selected Select All Select/Clear... Clear OK

Fixed Partial Pressure

Enter the value of log10(p)
(or for a range of values enter 'first last step') for
2 O2(g).

Press [Cancel] if the partial pressure is no longer fixed.

-8

OK

Cancel

Selection of Stoichiometric Solids from FToxicid

Selection - Equilib T(C) = 1250...

File Edit Show Sort

Selected: 55/190 Duplicates selected. SOLID So Page 20 Refresh

+	Code	Species	Data	Phase	T	V	Activity
	194	Pb ₂ Fe ₂₀₅ (s)	FACT53	solid	T	o	
	195	Pb ₂ FeSi ₂₀₇ (s)	FACT53	pb-fe_melilite		o	
	196	Pb ₂ Fe ₂₅ Si ₂₀₉ (s)	FACT53	melanotekite	T	o	
	197	Pb ₁₀ Fe ₂ Si ₂₀₁₇ (s)	FACT53	solid	T	o	
	198	PbZnSiO ₄ (s)	FACT53	solid	T	o	
	199	Pb ₂ ZnSi ₂₀₇ (s)	FACT53	pb-zn_melilite	T	o	
	200	Pb ₈ ZnSi ₆₀ O ₂₁ (s)	FACT53	solid	T	o	
+	201	SiO ₂ (s)	FToxicid	quartz(l)	T	V	0.1004
+	202	SiO ₂ (s2)	FToxicid	quartz(h)	V	V	0.3409
+	203	SiO ₂ (s3)	FToxicid	tridymite(l)	T	V	2.9347E-03
+	204	SiO ₂ (s4)	FToxicid	tridymite(h)	V	V	0.3616
+	205	SiO ₂ (s5)	FToxicid	cristobalite(l)	T	V	1.3080E-02
+	206	SiO ₂ (s6)	FToxicid	cristobalite(h)	V	V	0.3612
+	207	SiO ₂ (s7)	FToxicid	coesite	V	V	0.1604
+	208	SiO ₂ (s8)	FToxicid	stishovite	V	V	1.7984E-03
+	209	CaO(s)	FToxicid	lime	V	V	

Show Selected Select All Select/Clear... Clear OK

Selection of Solutions

File Units Parameters Help

T(C) P(atm) Energy(J) Mass(g) Vol(litre)

Reactants (7)

+ 100 Cu + <A> FeO + <100-A> SiO₂ + 0 CaO + 0.001 Pb + 0.001 Zn

Products

Compound species:

- + gas ideal real 38
- aqueous 0
- pure liquids 0
- * + pure solids 55

suppress duplicates

* - custom selection species: 93

Transitions - alpha <A>

Number of transitions:

Solution species

*	+	Base-Phase	Full Name
*	+	FToxic-SLAGA	ASlag-liq
		FToxic-SLAGB	BSlag-liq
		FToxic-SLAG?	?Slag-liq
*	+	FToxic-SPINA	ASpinel
		FToxic-MeO_A	AMonoxide
!	FToxic-MeO_?	?Monoxide	
!	FToxic-cPyr	Clinopyroxene	
!	FToxic-oPyr	Orthopyroxene	

Custom Solutions

- 1 fixed activities
- 0 ideal solutions
- 0 activity coefficients

Pseudonyms

apply

include molar volumes

Total Species (max 1500) 205
Total Solutions (max 40) 17

Final Conditions

<A>		T(C)	P(atm)	Product H(J)
10 90		1250	1	

10 steps Table

Equilibrium

normal normal + transitions
 transitions only open
 predominant

FactSage 6.2 beta g:\CAD\...\metall-saturated\EquiCu-Mt-SI_01.DAT

ASlag or ?Slag
?Monoxide
Dormant phases

Calculate transitions

Transitions

Results - Equilib A=10 (page 1/4) FactSage 6.2 be... - □ X

Output Edit Show Pages T(C) P(atm) Energy(J) Mass(g) Vol(litre)

A=10 | A=63.2736 | A=81.769 | A=90 |

```
+ 106.41 gram Cu-liq_or_speiss
(106.41 gram, 1.7060 mol)
(1250.00 C, 1 atm, a=1.0000)
( 6.5704E-04 wt.-% Pb
+ 98.087 wt.-% Cu
+ 3.9339E-02 wt.-% Fe
+ 1.8552 wt.-% S
+ 9.2040E-05 wt.-% Zn
+ 1.7374E-02 wt.-% O
FTmisc
FTmisc
FTmisc
FTmisc
FTmisc
FTmisc
FTmisc)
```

System component	Mole fraction	Mass fraction
Pb	1.9779E-06	6.5704E-06

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

```
0 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
+ 0.57238 wt.-% Fe
+ 80.038 wt.-% Cu
+ 6.4079E-05 wt.-% Zn
+ 1.7725E-04 wt.-% Pb
FTmisc
FTmisc
FTmisc
FTmisc
FTmisc
FTmisc)
```

System component	Mole fraction	Mass fraction
Pb	4.5638E-07	1.7725E-06
Zn	5.2279E-07	6.4079E-07
Cu	0.67195	0.80038
Fe	5.4678E-03	5.7238E-03
S	0.32259	0.19389

```
+ 15.437 gram ASlag-liq#1
(15.437 gram, 0.21857 mol)
(1250.00 C, 1 atm, a=1.0000)
( 35.129 wt.-% SiO2
+ 54.903 wt.-% FeO
+ 5.4485 wt.-% Fe2O3
+ 9.3912E-04 wt.-% PbO
+ 6.7716E-03 wt.-% ZnO
+ 4.1536 wt.-% Cu2O
+ 0.14512 wt.-% SiS2
+ 0.18082 wt.-% FeS
+ 1.9091E-02 wt.-% Fe2S3
+ 2.7096E-06 wt.-% PbS
+ 2.1824E-05 wt.-% ZnS
+ 1.2435E-02 wt.-% Cu2S
FToxid
FToxid)
```

A Series of Calculations

◀ Menu - Equilib: comments

File Units Parameters Help

T(C) P(atm) Energy(J) Mass(g) Vol(litre)

Reactants (7)

+ 100 Cu + <A> FeO + <100-A> SiO₂ + 0 CaO + 0.001 Pb + 0.001 Zn

Products

Compound species

- + gas ideal real 38
- aqueous 0
- pure liquids 0
- * + pure solids 55
- suppress duplicates
- * - custom selection species: 93

Solution species

*	+	Base-Phase	Full Name
	I	FToxic-SLAGA	ASlag-liq
		FToxic-SLAGB	BSlag-liq
		FToxic-SLAG?	?Slag-liq
	+	FToxic-SPINA	ASpinel
		FToxic-MeO_A	AMonoxide
	!	FToxic-MeO_?	?Monoxide
	!	FToxic-cPyr	Clinopyroxene
	!	FToxic-oPyr	Orthopyroxene

Custom Solutions

- 1 fixed activities
- 0 ideal solutions
- 0 activity coefficients

Pseudonyms

apply

include molar volumes

Total Species (max 1500) 205
Total Solutions (max 40) 17

Target: - none -

Estimate ALPHA: .6

Mass(g): 0

Legend

- I - immiscible 1
- ! - dormant 12
- + - selected 3

Show all selected

species: 112
solutions: 17

Default

Final Conditions

<A>		T(C)	P(atm)	Product H(J)
63.821		1250	1	

10 steps Table 20 calculations

Equilibrium

normal normal + transitions
 transitions only open
 predominant

FactSage 6.2 beta g:\CAD\...\metall-saturated\EquiCu-Mt-SI_01.DAT

Output Results in Excel

Results - Equilib A=63 (page 1/20) FactSage 6.2 b...

Output Edit 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> FeO + <100-A> SiO₂ +

(gram) 0 CaO + 0.001 Pb + 0.001 Zn =

+ 0.81356 02

0.00000

Output

Page Range

All 20 pages
 Current page 1

Type of Output

Printer Printer setup ...
 Text file (*.txt)
 Equilib Results File (Equi*.res)
 Xml file (*.xml)
 Excel Spreadsheet
 Open Text Spreadsheet
 Save Text Spreadsheet
 Swap rows & columns

OK

FACT53
FACT53
FACT53
FACT53
FACT53

+ 5.4928E-10	0	FACT53
+ 3.1404E-10	FeO	FACT53
+ 2.2758E-10	CuO	FACT53
+ 7.8362E-11	SiO	FACT53
+ 4.9120E-11	FeS	FACT53

Select Species for Output

Results - Equilib A=63 (page 1/20) FactSage 6.2 b... X

Output Edit Show Pages

T(C) P(atm) Energy(J) Mass(g) Vol(litre)

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> FeO + <100-A> SiO₂ +

(gram) 0 CaO + 0.001 Pb + 0.001 Zn =

+ 0.1 Spreadsheet Setup

System Properties

Property columns: 2

Column:	- 1 -	- 2 -
Variable:	Alpha	T(C)

Species Properties

Columns per species: 1

order species order props.

Column:	- 1 -
Variable:	Wt%

Species

Columns: 7

Select ...

Species: 5

Cancel

Default

OK

+ 3.1404E-10 FeO FACT53
+ 2.2758E-10 CuO FACT53
+ 7.8362E-11 SiO FACT53
+ 4.9120E-11 FeS FACT53

Fe-Zn-Si-O System

Spreadsheet - Equilib T(C) = 1...

File Edit Show

Selected: 5/225 Spreadsheet Species Page 1 Refresh

+	Code	Species	Data	Phase	T	V	Activity
+	272	Pb(CuLQ)	FTmisc	FTmisc-CuLQ			5.1975E-06
	273	Cu(CuLQ)	FTmisc	FTmisc-CuLQ			0.9767
	274	Fe(CuLQ)	FTmisc	FTmisc-CuLQ			6.2170E-03
	275	Si(CuLQ)	FTmisc	FTmisc-CuLQ			8.4239E-05
	276	Zn(CuLQ)	FTmisc	FTmisc-CuLQ			1.8842E-08
	277	O(CuLQ)	FTmisc	FTmisc-CuLQ			4.3782E-05
	286	S(MATT)	FTmisc	FTmisc-MATT			8.3687E-05
	287	Fe(MATT)	FTmisc	FTmisc-MATT			6.2170E-03
	288	Cu(MATT)	FTmisc	FTmisc-MATT			0.6014
	289	Zn(MATT)	FTmisc	FTmisc-MATT			1.8842E-08
+	290	Pb(MATT)	FTmisc	FTmisc-MATT			5.1978E-06
+	313	SiO ₂ (SLAGA)	FToxid	FToxid-SLAGA			0.8350
	314	CaO(SLAGA)	FToxid	FToxid-SLAGA			

'+' denotes all the Species Properties as defined in the Spreadsheet Setup.

Select All Clear OK

Spreadsheet - Equilib T(C) = 1...

File Edit Show

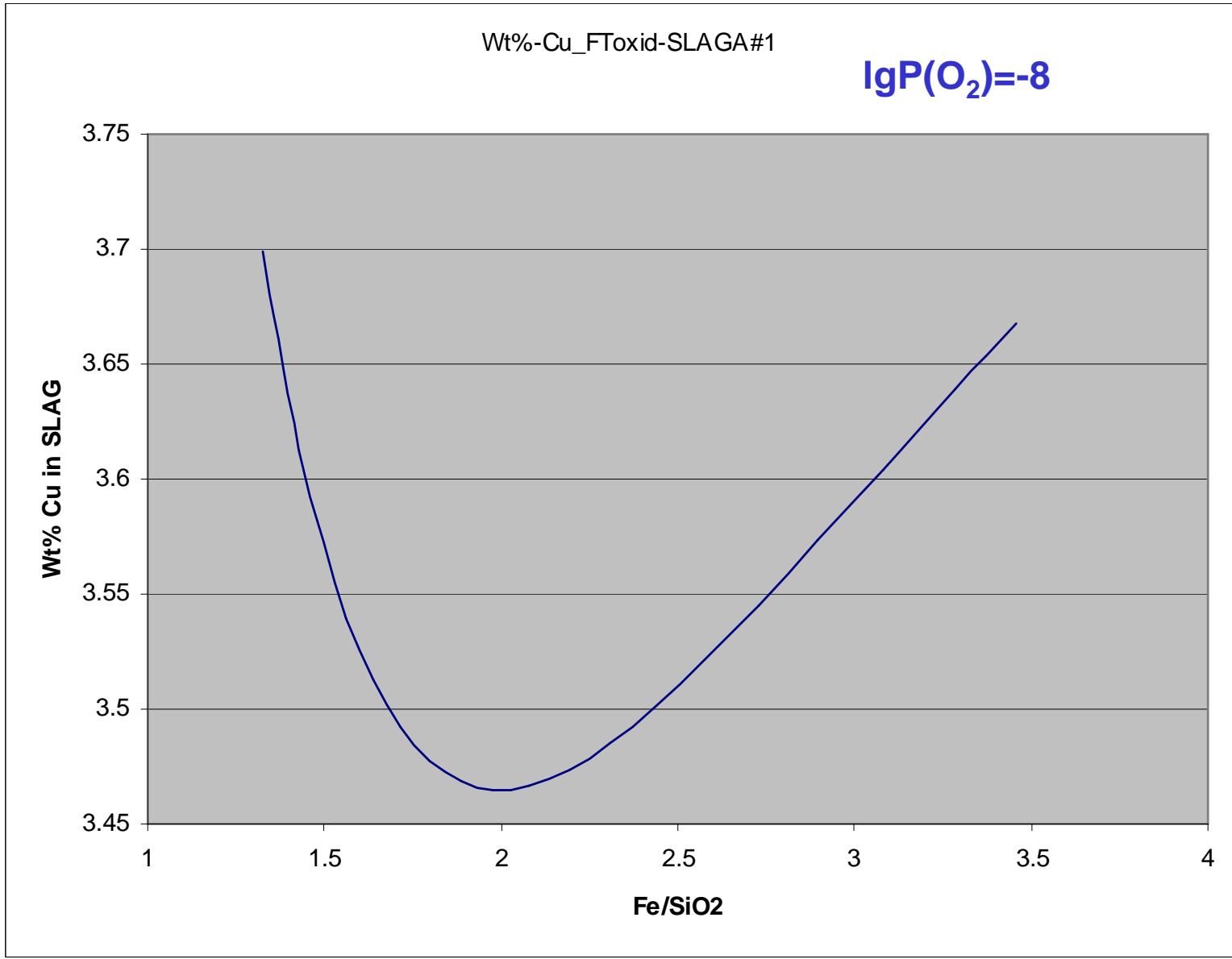
Selected: 5/225 Spreadsheet Species Page 1 Refresh

+	Code	Species	Data	Phase	T	V	Activity
	509	All Elements		FTmisc-MATT			
+	520	All Elements		FToxid-SLAGA#1			
	523	All Elements		FToxid-SPINA			
	525	All Elements		FToxid-MeO_?			
	526	All Elements		FToxid-cPyr			
	527	All Elements		FToxid-oPyr			
	528	All Elements		FToxid-wOLLA			
	529	All Elements		FToxid-bC2S			
	530	All Elements		FToxid-aC2S			
	531	All Elements		FToxid-Mel_			
	532	All Elements		FToxid-OlivA			
	533	All Elements		FToxid-ZNIT			
	534	All Elements		FToxid-wILL			
	535	All Elements		FToxid-PbO_			
	536	All Elements		FToxid-PCSi			

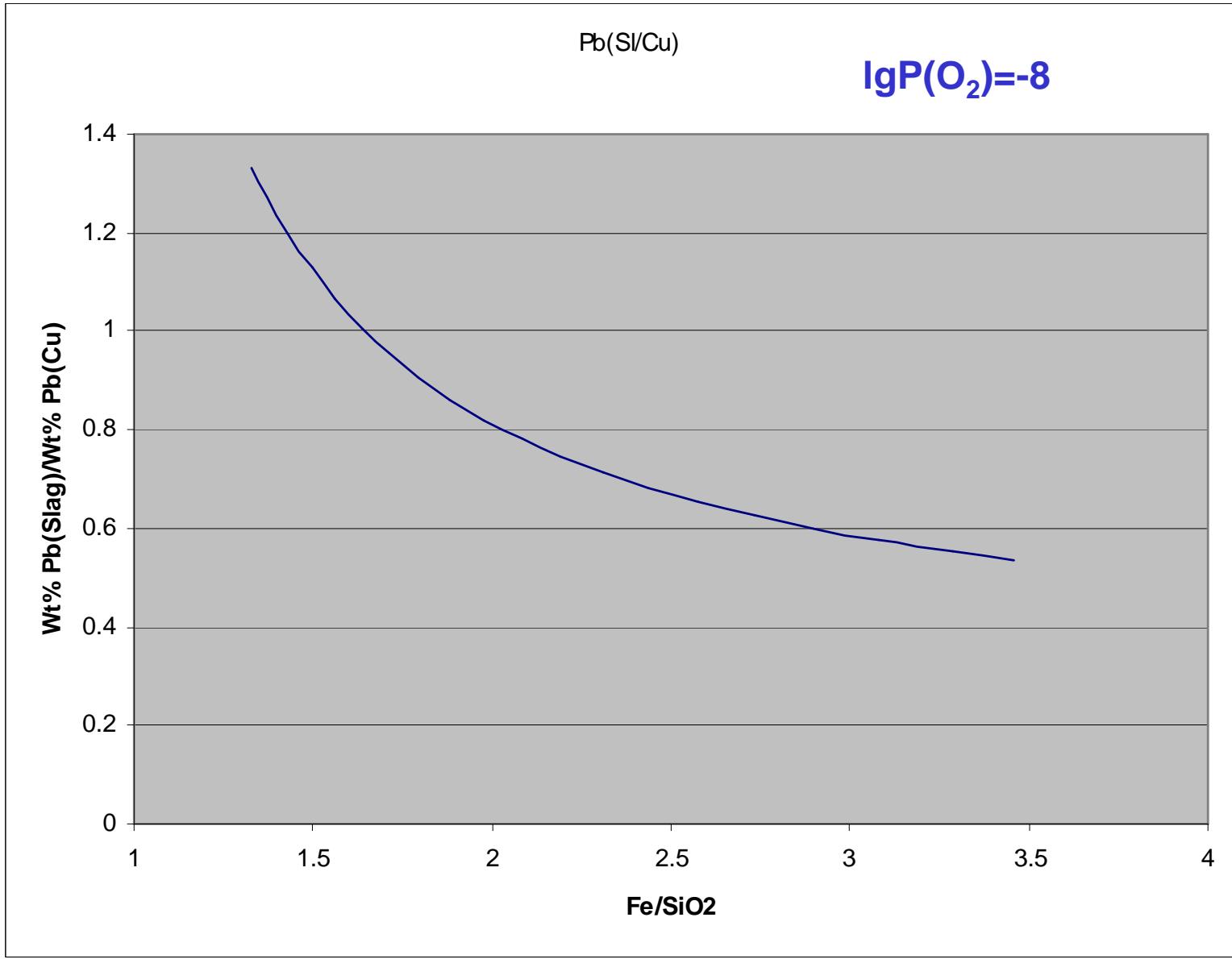
'+' denotes all the Species Properties as defined in the Spreadsheet Setup.

Select All Clear OK

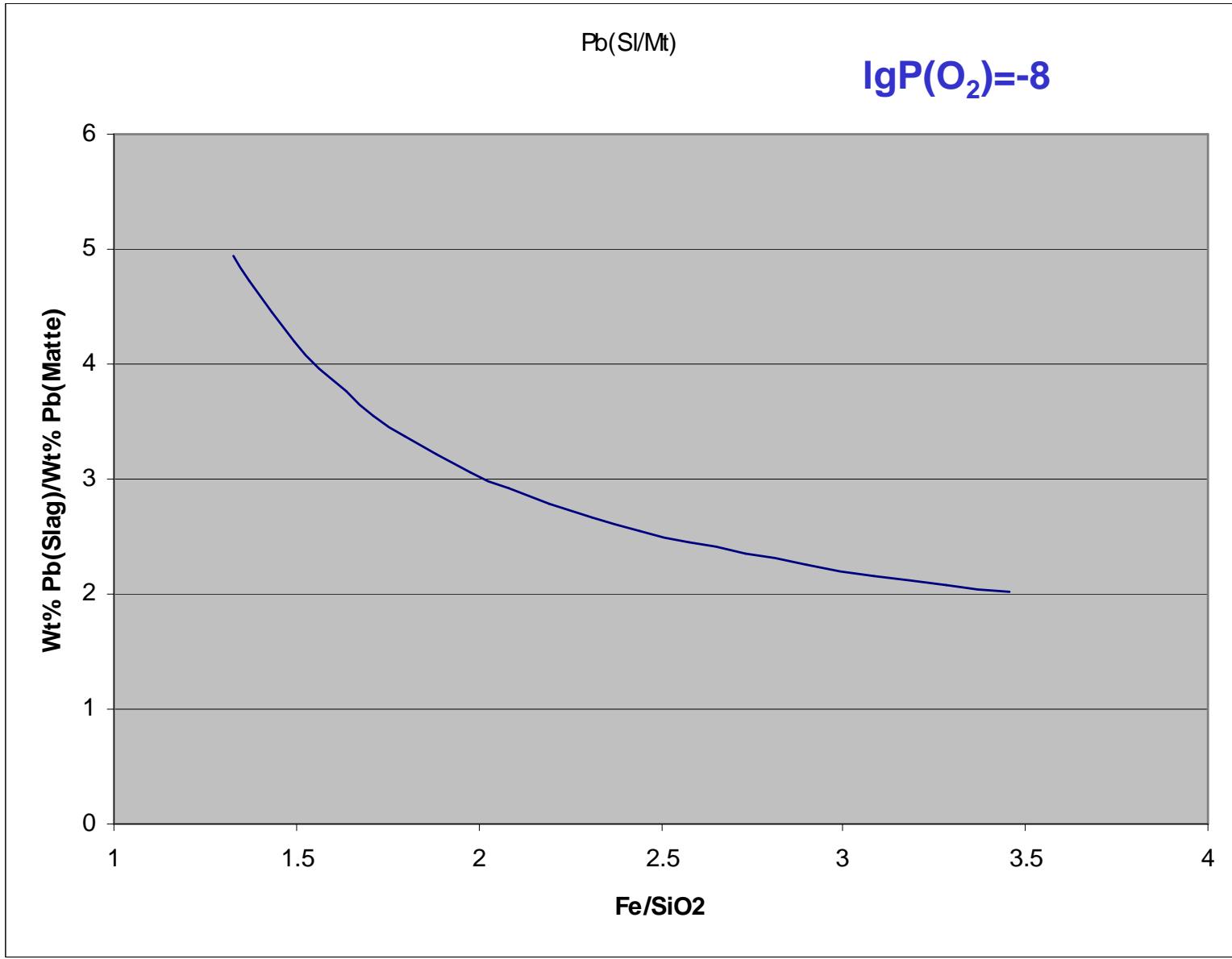
Cu losses to Slag



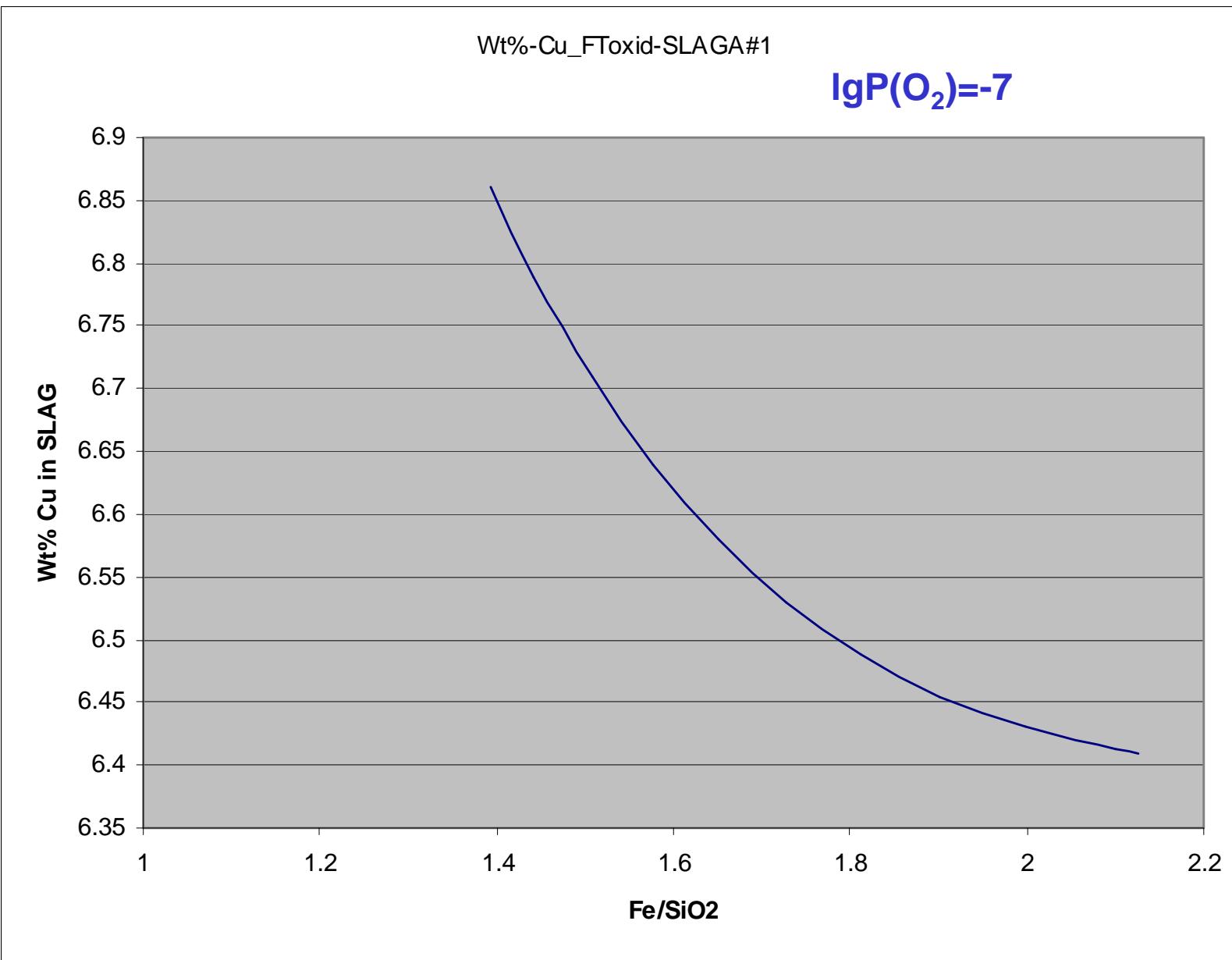
Distribution of Pb between Slag and Cu



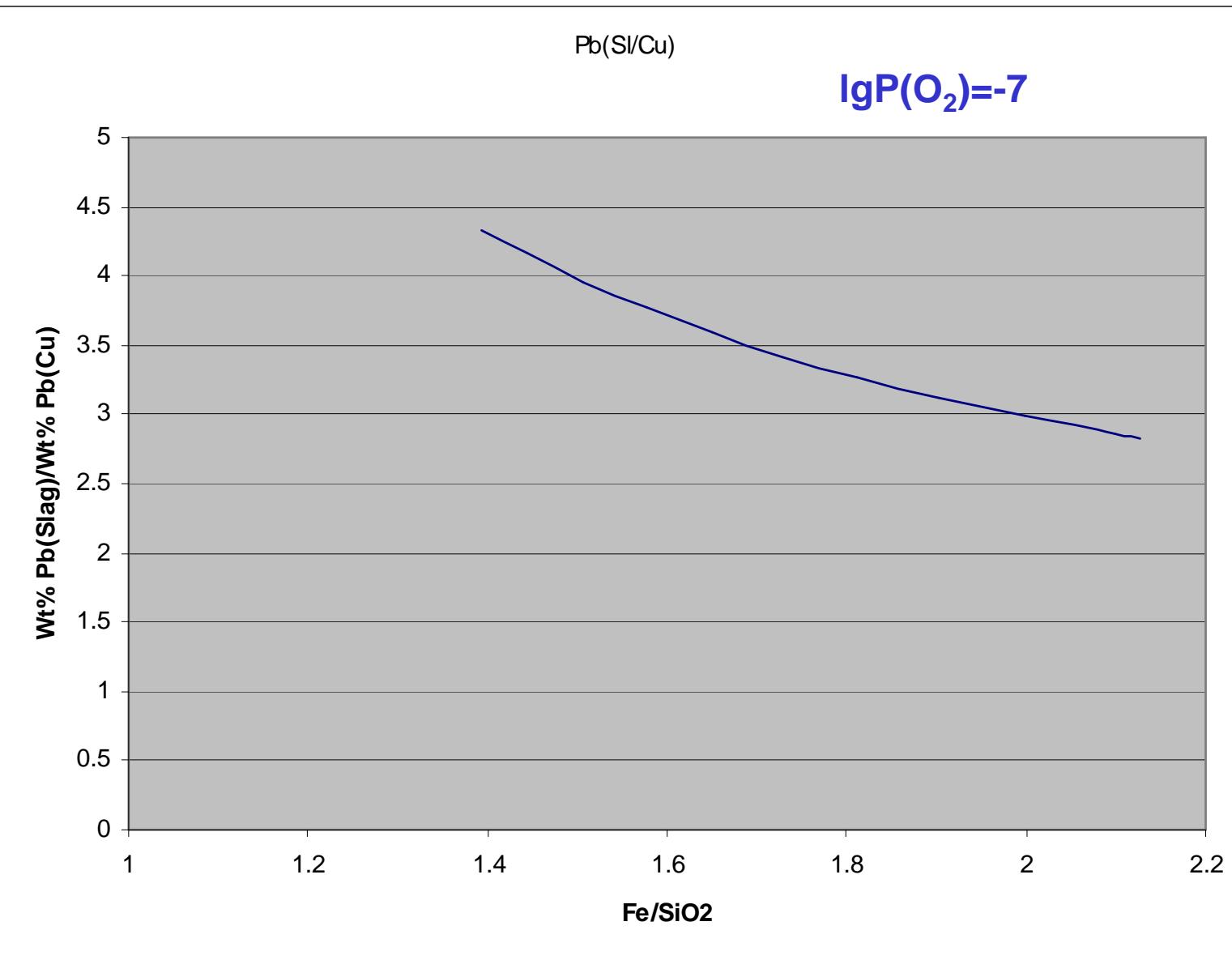
Distribution of Pb between Slag and Matte



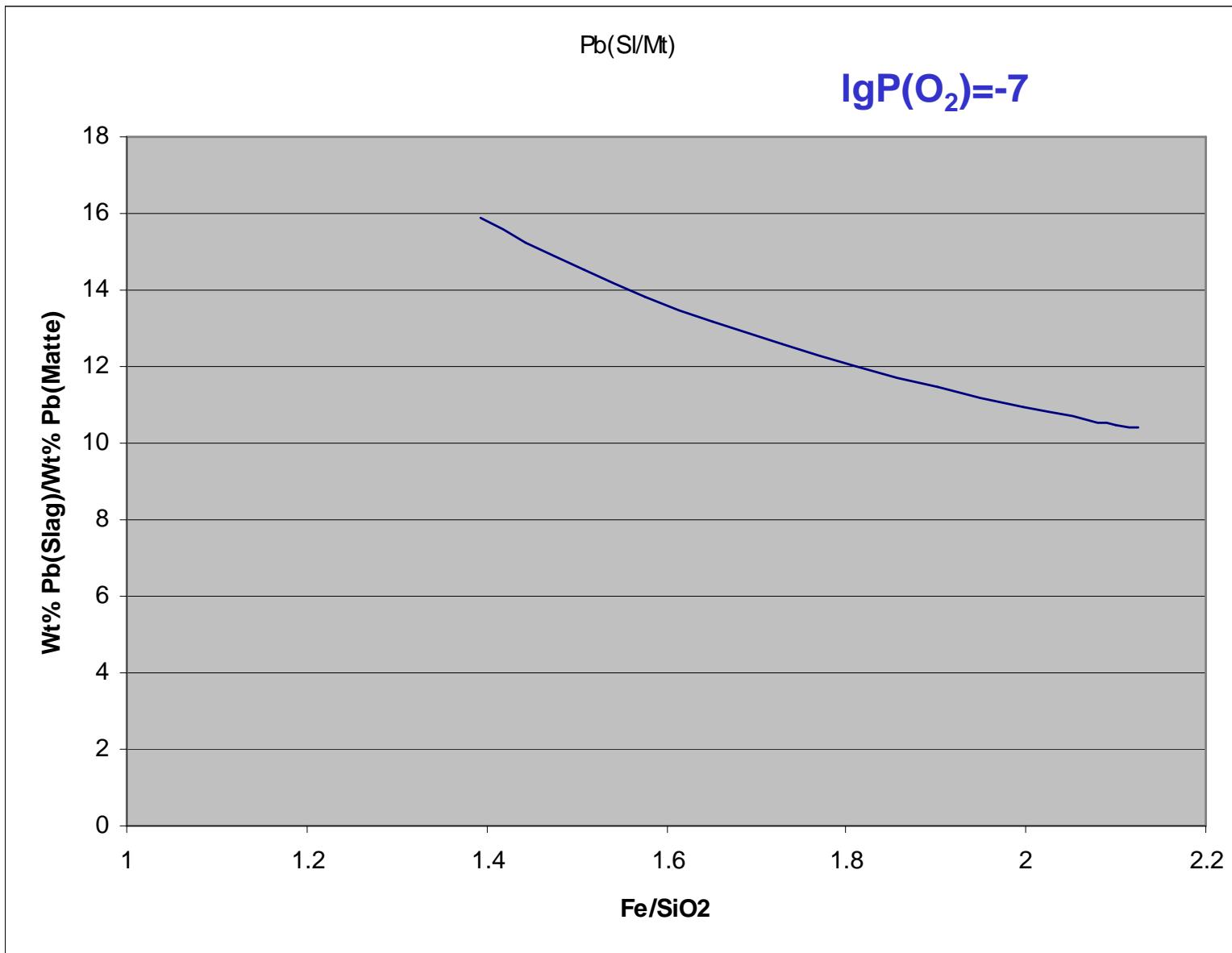
Cu losses to Slag



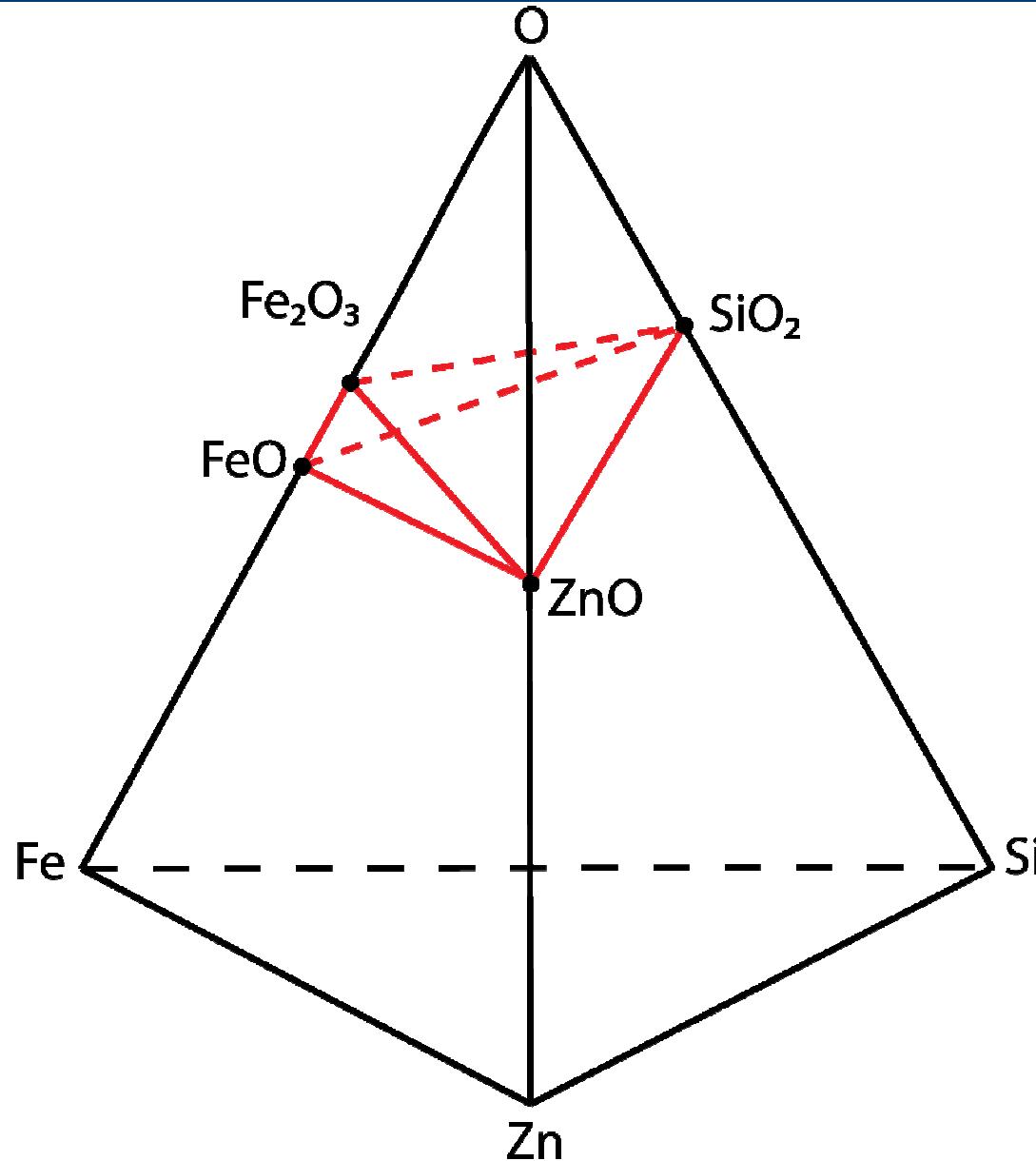
Distribution of Pb between Slag and Cu



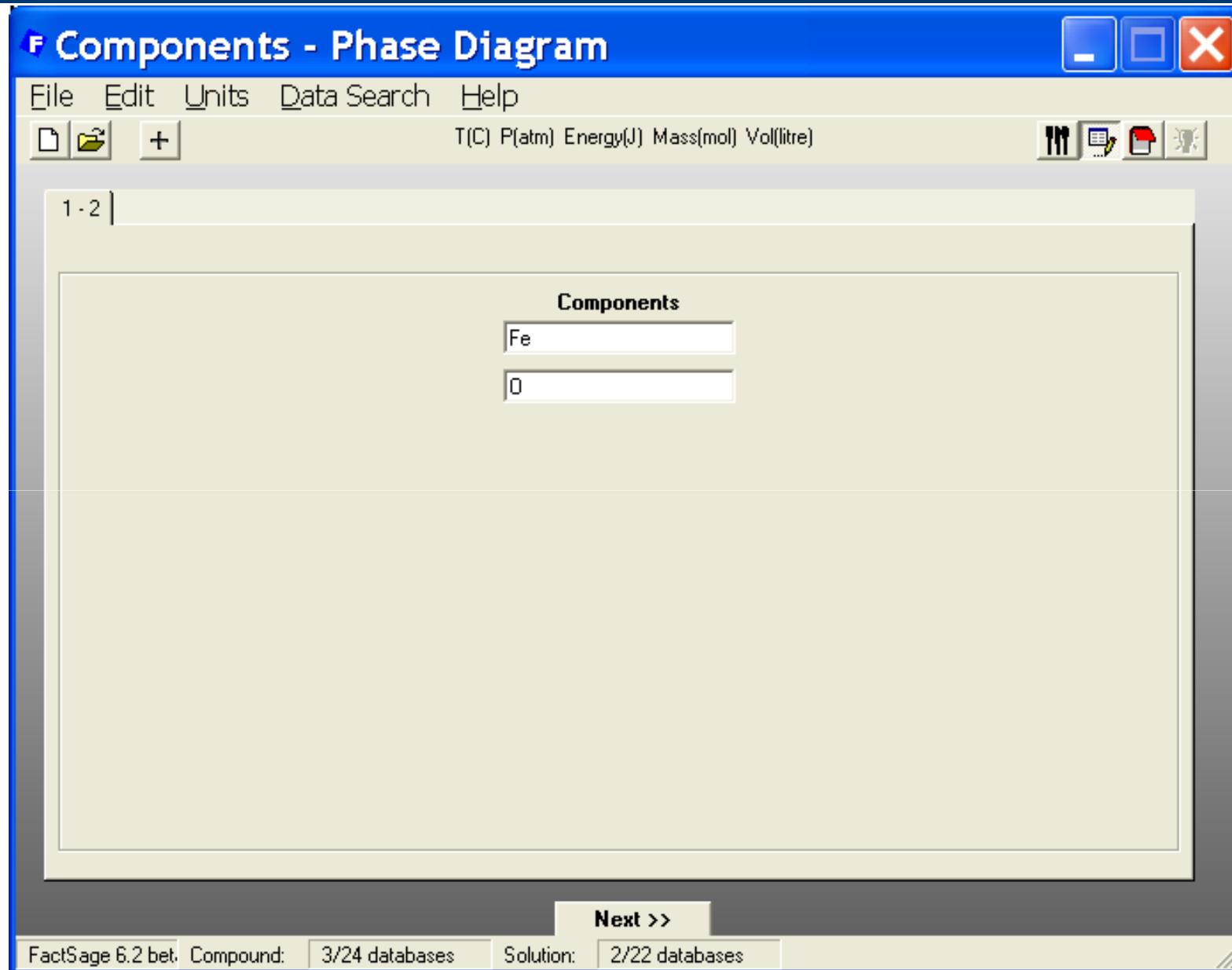
Distribution of Pb between Slag and Matte



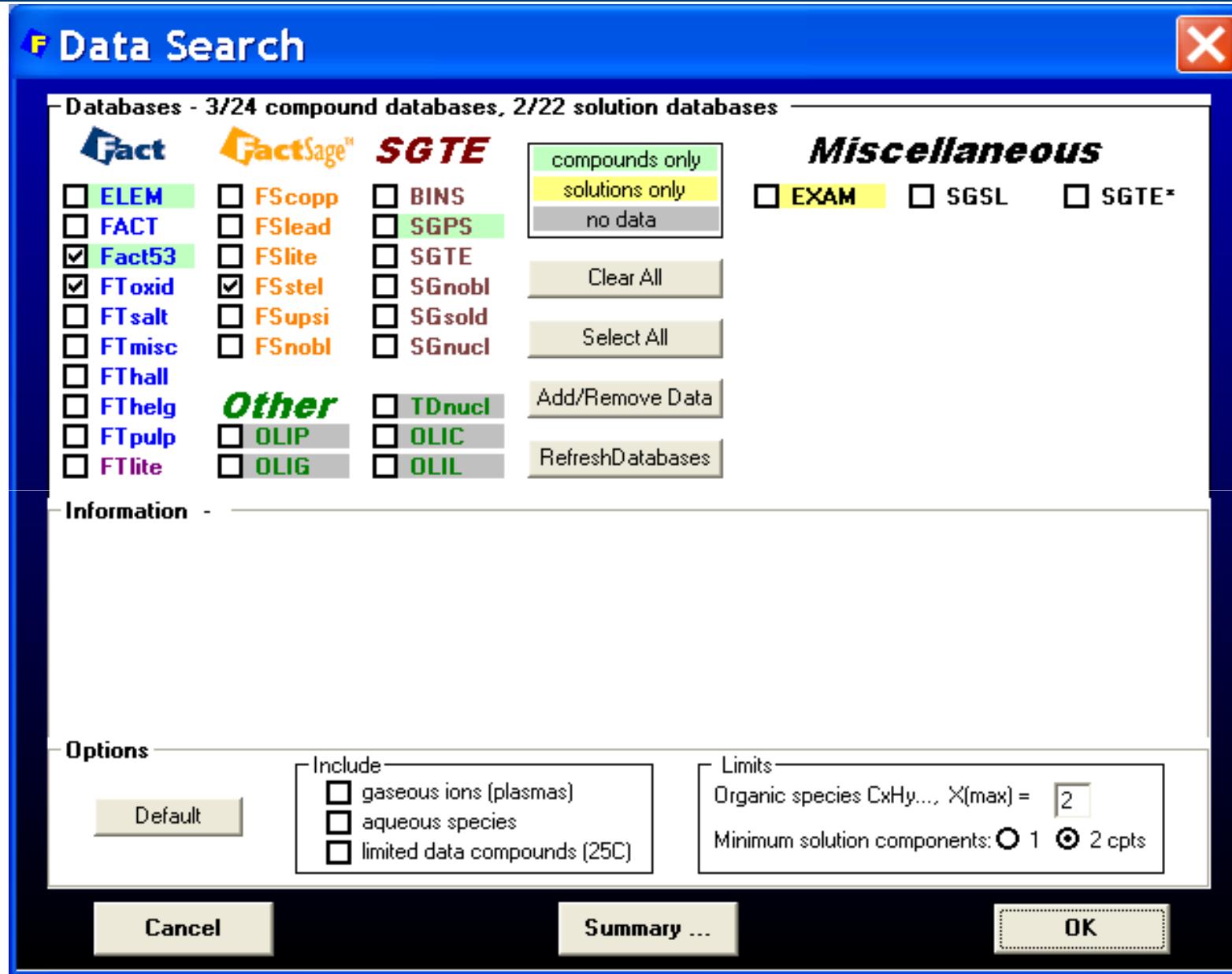
Fe-Zn-Si-O System



Fe-O System



Fe-O System



Fe-O System

F Selection - Equilib

File Edit Show Sort
Selected: 5/18 Duplicates selected SOLID Sorted by Code

+	Code	Species	Data	Phase	T	V	Activity
	15	Fe2O3(s2)	FACT53	high-pressure-he...	V		
	16	Fe2O3(s3)	FACT53	high-pressure-he...	V		
	17	Fe3O4(s)	FACT53	magnetite	V		
	18	Fe3O4(s2)	FACT53	magnetite	V		
	19	Fe3O4(s3)	FACT53	high-pressure-m...	V		
	20	Fe3O4(s4)	FACT53	high-pressure-m...	V		
+	21	Fe(s)	FSstel	bcc_a2			
+	22	Fe(s2)	FSstel	fcc_a1			
	23	Fe2O3(s)	FSstel	hematite	V		
	24	Fe3O4(s)	FSstel	magnetite	V		
	25	Fe3O4(s2)	FSstel	magnetite	V		
+	26	Fe2O3(s)	FToxid	hematite	V		
+	27	Fe2O3(s2)	FToxid	high-pressure-he...	V		
+	28	Fe2O3(s3)	FToxid	high-pressure-he...	V		

Show Selected Select All Select/Clear... Clear OK

include molar volumes
Total Species (max 1500) 24
Total Solutions (max 40) 5

Default

Legend
I - immiscible 1
+ - selected 3
Show all selected
species: 14 solutions: 5 Select

Target
- none -
Estimate T(K): 1000
Mass(mol): 0

Variables
T(C) O/(Fe+O)
400 1800 0.1
T(C) vs O/(Fe+O)

FactSage 6.2 beta g:\CAD\...\metall-saturated\PhasFe-O_1atm.DAT

Phase Diagram
Y X Calculate >

Fe-O System

Variables: Fe-O T(C) vs composition #1.



Variables

Y
X

compositions

$\log_{10}(a)$

A
B C

Y steps:
X steps:

Next >>

T and P

Temperature

T(C)
 1/TK

Y-axis
Max:
Min:

Pressure

P(atm)
 log P

constant

Compositions (mole)

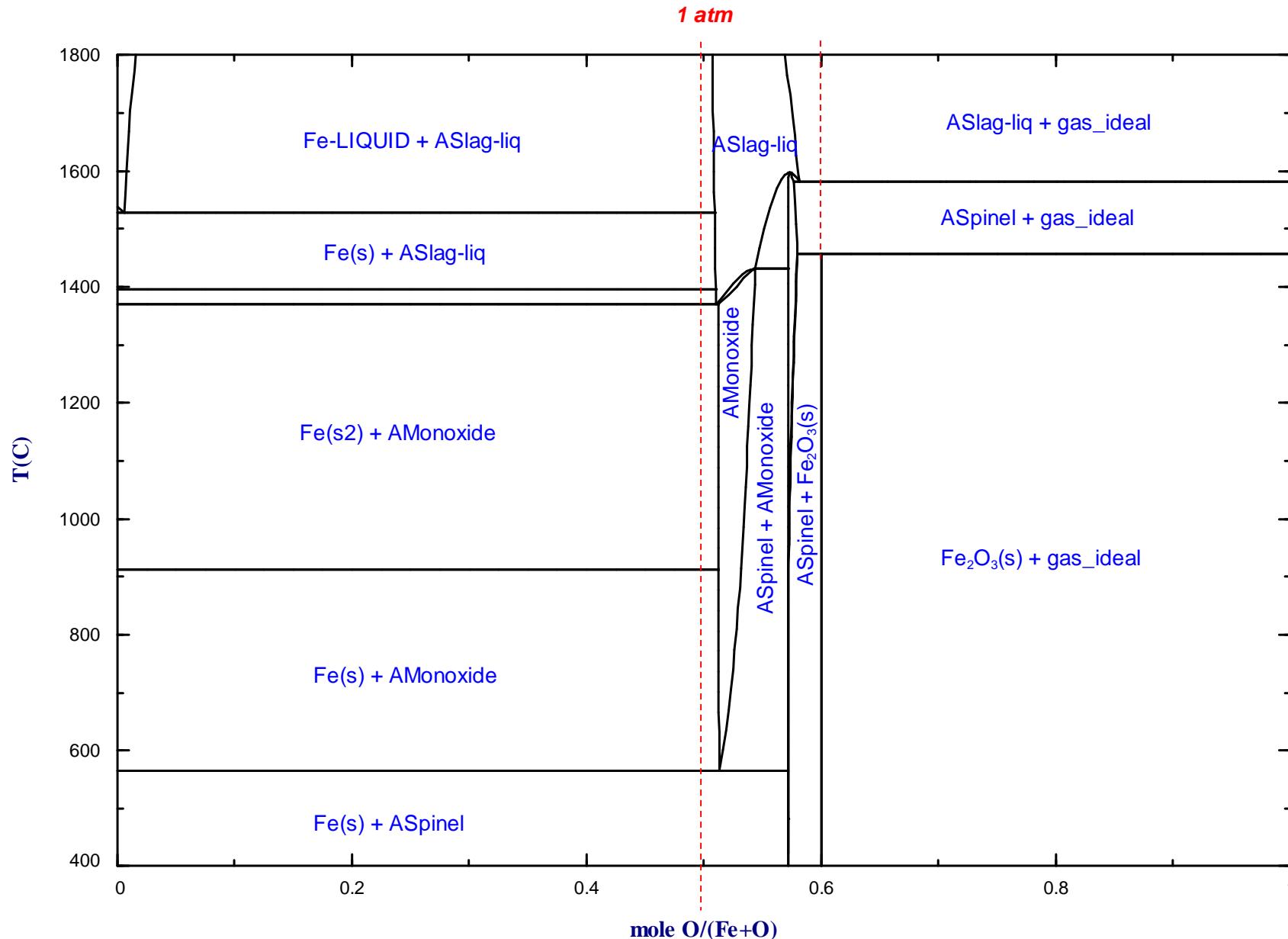
#1. $\frac{0 \text{ Fe} + 1 \text{ O}}{1 \text{ Fe} + 1 \text{ O}} =$ X-axis

1 (max)
0 (min)

Cancel

OK

Fe-O System



Fe-O System

Variables: Fe-O T(C) vs composition #1.



Variables

Y
X

compositions

$\log_{10}(a)$

A

C

Y steps:
X steps:

Next >>

T and P

Temperature

T(C)
 1/T(K)

Y-axis
Max:
Min:

Pressure

P(atm)
 log P

constant

Compositions (mole)

#1. $\frac{0}{1} \text{ Fe} + \frac{1}{1} \text{ O} = \frac{1}{1} \text{ Fe} + \frac{1}{1} \text{ O}$

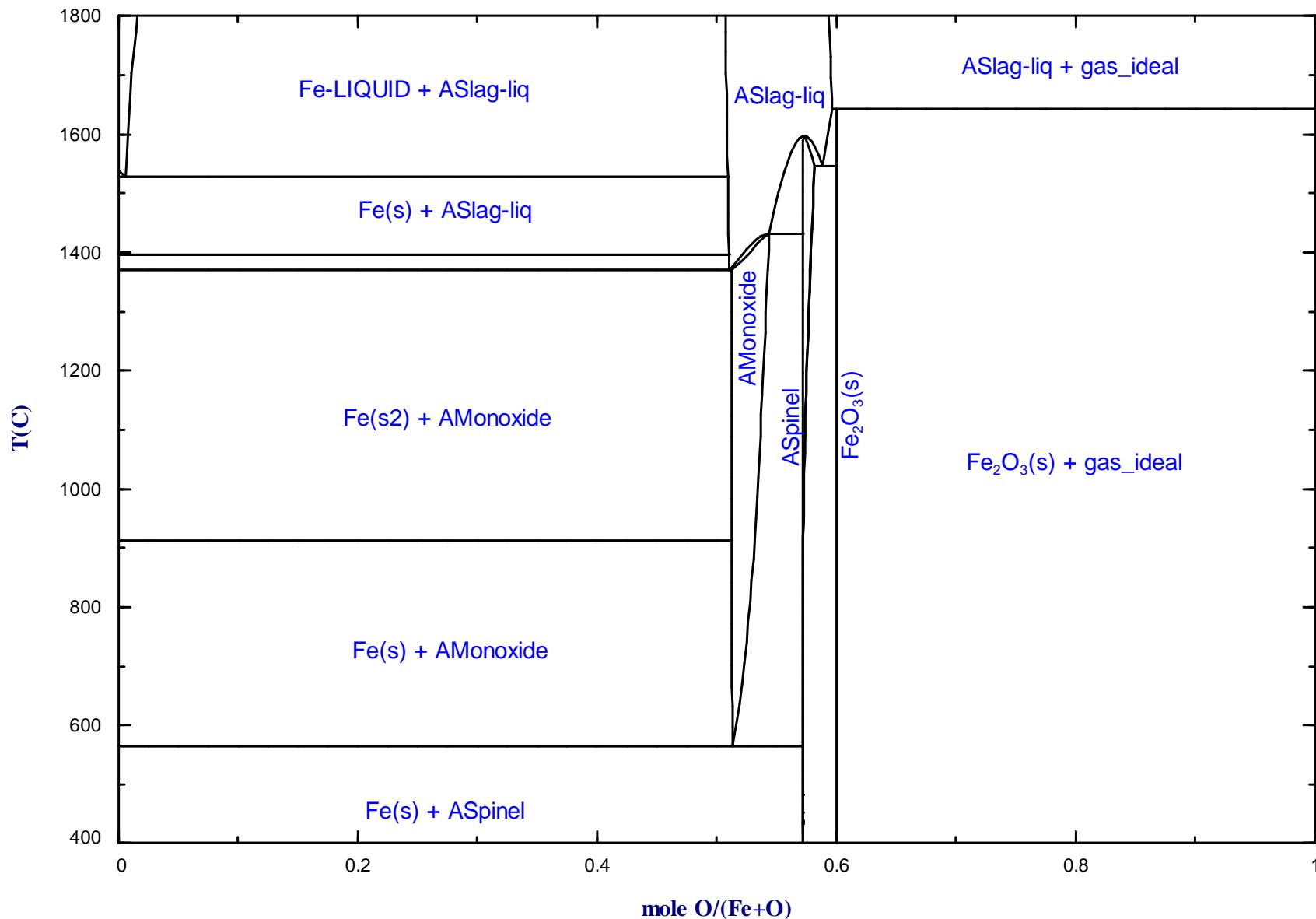
X-axis
1 (max)
0 (min)

Cancel

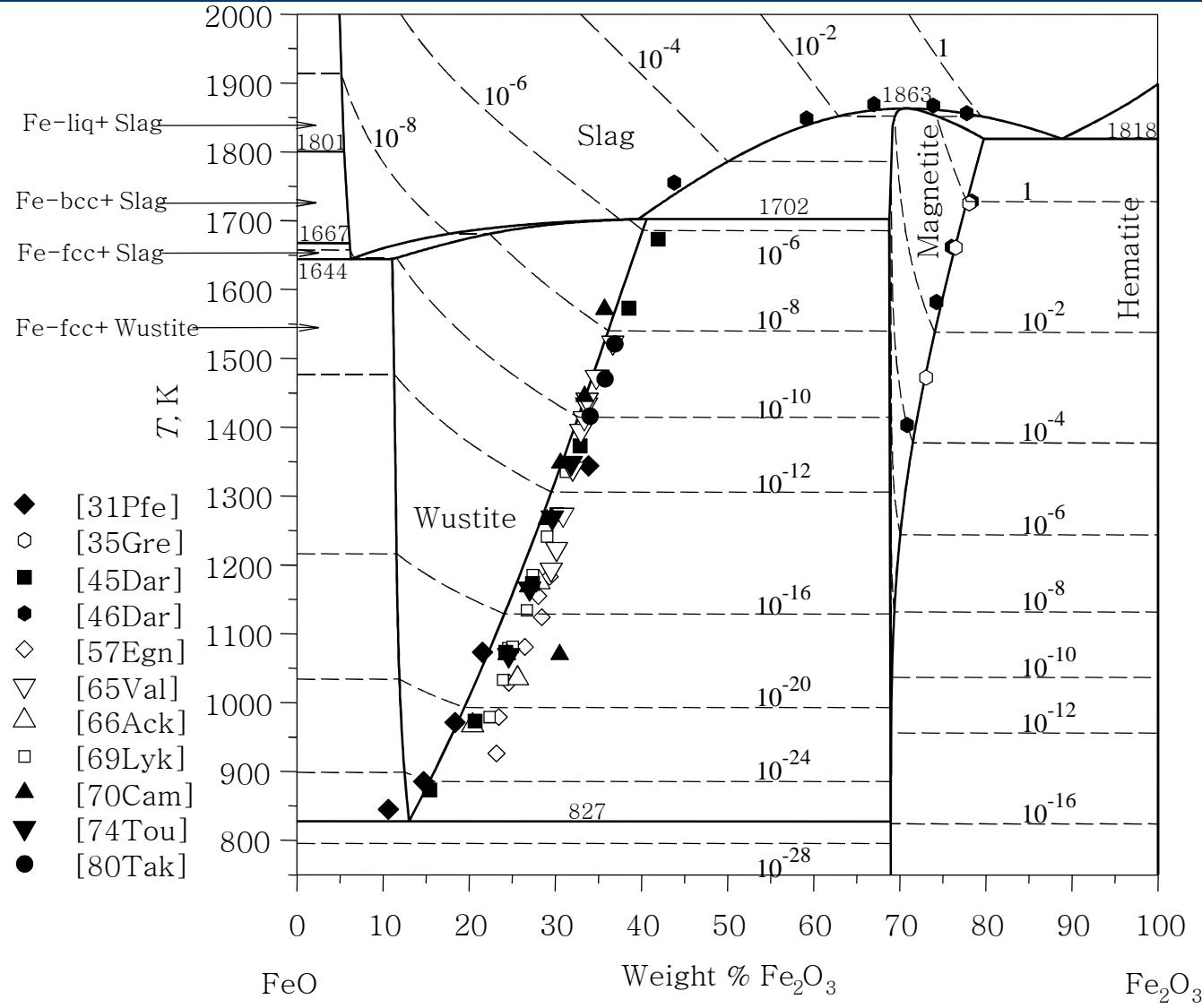
OK

Fe-O System

P=10000 atm



Fe-O System



FeO- Fe_2O_3 phase diagram: experimental points and calculated lines.
Dashed lines are oxygen isobars (atm).

Fe-Zn-O System

Components - Phase Diagram

File Edit Units Data Search Help

T(C) P(atm) Energy(J) Mass(mol) Vol(litre)

1 - 3

Components

Fe
Zn
O

FactSage Data Search

Databases - 3/24 compound databases, 2/22 solution databases

Fact FactSage™ SGTE Miscellaneous

ELEM FScopp BINS compounds only
FACT FSlead SGPS solutions only
Fact53 FSlite SGTE no data
FToxid FSstel SGnobl
FTsalt FSupsi SGsold
FTmisc FSnobl SGnucl
FThall TDnucl
FThelg OLIP OLIC
FTpulp OLIG OLIL
FTlite

Clear All
Select All
Add/Remove Data
RefreshDatabases

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 database click-mouse-right-button (note, this is NOT recommended).

If database is stored on your PC but not listed here then you must 'add the database to the list' - click on 'Add/Remove ...'.

Options

Include

Default

gaseous ions (plasmas)
aqueous species (✓)
limited data compounds (25C)

Limits

Organic species CxHy..., X(max) = [2]
Minimum solution components: 1 2 cpts

Cancel Summary ... OK

FactSage 6.2 beta Compound: 3/24 databases Solution: 2/22 databases Next >

Fe-Zn-O System

F Menu - Phase Diagram: Only O₂ gas species is selected

File Units Parameters Variables Help

T(C) P(atm) Energy(J) Mass(mol) Vol(litre)

Components (3)

Fe + Zn + O

Products

Compound species

- * gas ideal real 1
- aqueous 0
- pure liquids 0
- * pure solids 7
- suppress duplicates
- * - custom selection species: 8

Target

- none -

Estimate T(K):

Mass(mol):

Solution species

	Base-Phase	Full Name
*	FSstel-FEZ1	FEZN4
+	FSstel-FEZ2	FEZN_DELTA
+	FSstel-FEZ3	FEZN_ZETA
+	FSstel-HCP	HCP_A3:Me2(C,N)
I	FToxid-SLAGA	ASlag-liq
+	FToxid-SPINA	ASpinel
+	FToxid-MeO_A	AMonoxide
+	FToxid-ZNIT	Zincite

Legend

- I - immiscible 1
- + - selected 12

Show all selected

species: 51 solutions: 14

Variables

T(C)	O/(Fe+Zn+O)	Zn/(Fe+Zn+O)		
1500	0.1	0.1		

A = O, B = Fe, C = Zn

FactSage 6.2 beta g:\...\PhasFe-Zn-O_1500-C_O2-gas.DAT

F Selection - Equilib

File Edit Show Sort

Selected: 7/23 Duplicates selected SOLID Sorted by Code

	Code	Species	Data	Phase	T	V	Activity
+	25	Fe3O4(s4)	FACT53	high-pressure-m...			
+	26	Zn(s)	FACT53	solid			
+	27	ZnO(s)	FACT53	zincite			
+	28	ZnFe2O4(s)	FACT53	solid			
+	29	Fe(s)	FSstel	bcc_a2			
+	30	Fe(s2)	FSstel	fcc_a1			
+	31	Fe2O3(s)	FSstel	hematite	V		
+	32	Fe3O4(s)	FSstel	magnetite	V		
+	33	Fe3O4(s2)	FSstel	magnetite	V		
+	34	Zn(s)	FSstel	hcp_zn	o		
+	35	Fe2O3(s)	FToxid	hematite	V		
+	36	Fe2O3(s2)	FToxid	high-pressure-he...	V		
+	37	Fe2O3(s3)	FToxid	high-pressure-he...	V		
+	38	ZnO(s)	FToxid	zincite			

Show Selected Select All Select/Clear... Clear OK

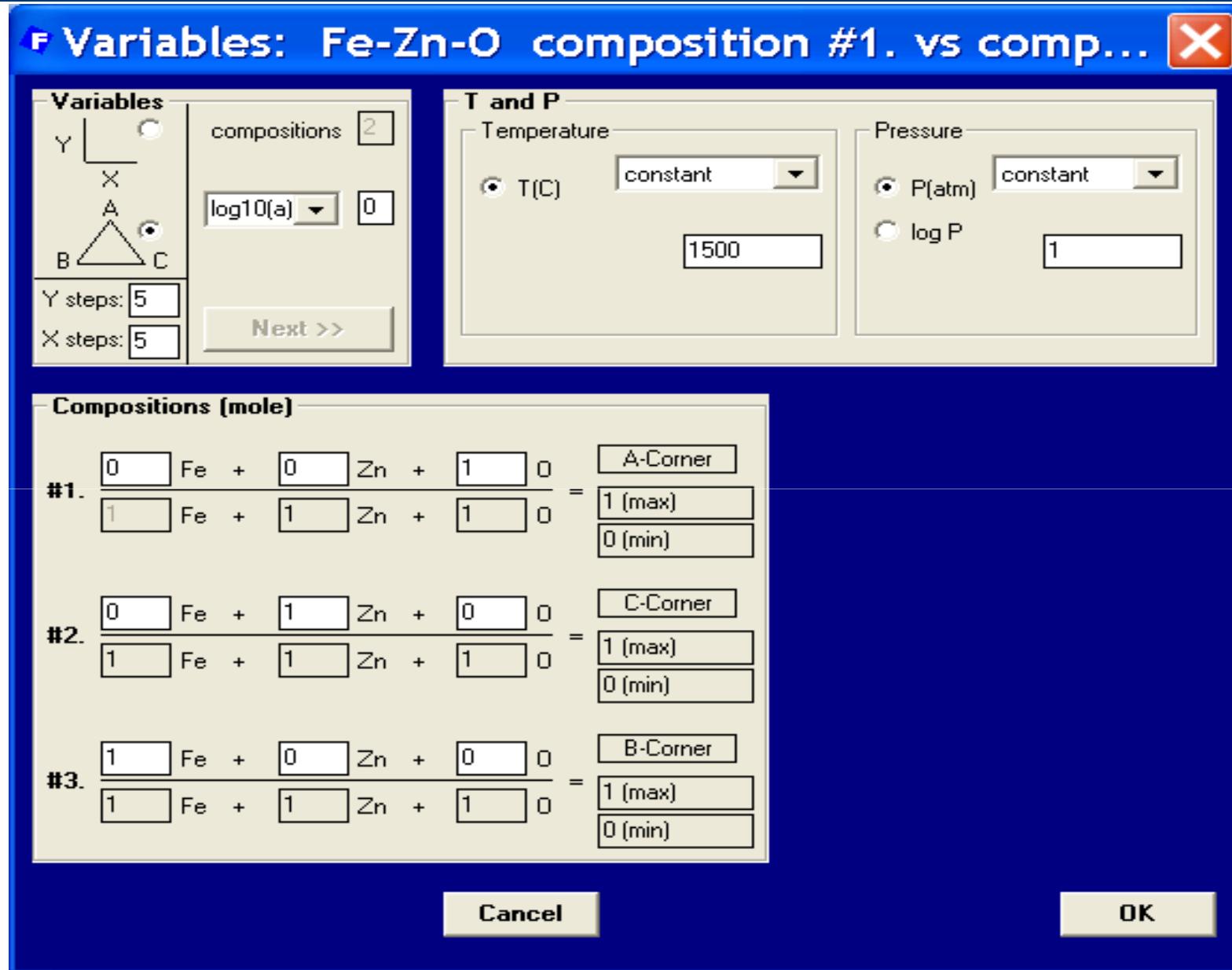
Pseudonyms apply List ...

include molar volumes

Total Species (max 1500) 59
Total Solutions (max 40) 14

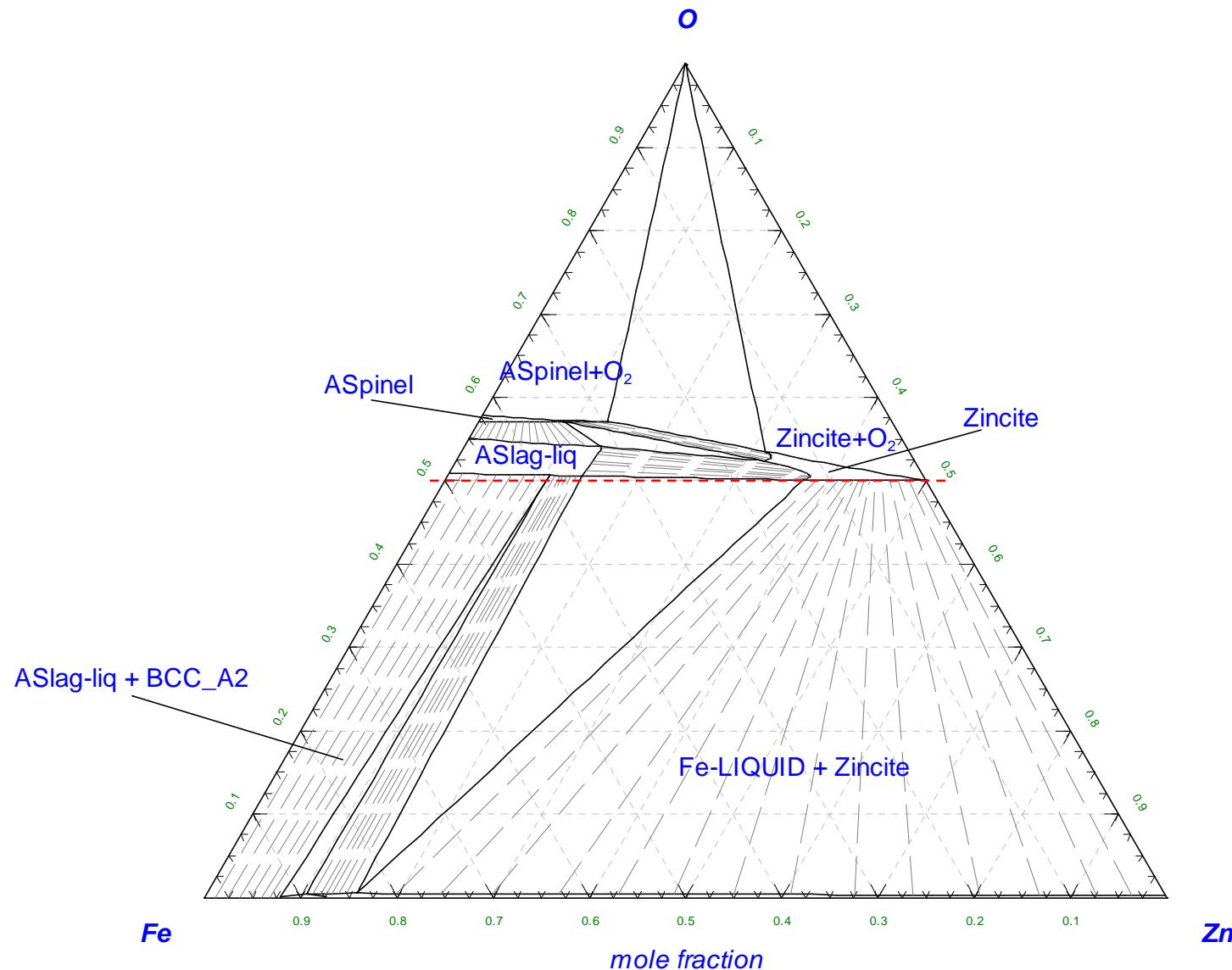
Default

Fe-Zn-O System



Fe-Zn-O System

1500°C



FeO-ZnO System (oxide phases only)

Components - Phase Diagram

File Edit Units Data Search Help

T(C) P(atm) Energy(J) Mass(mol) Vol(litre)

1 - 2

Components

FeO
ZnO

Data Search

Databases - 1/24 compound databases, 1/22 solution databases

Fact **FactSage™** **SGTE**

<input type="checkbox"/> ELEM	<input type="checkbox"/> FSopp	<input type="checkbox"/> BINS	compounds only
<input type="checkbox"/> FACT	<input type="checkbox"/> FLead	<input type="checkbox"/> SGPS	solutions only
<input type="checkbox"/> Fact53	<input type="checkbox"/> FSlite	<input type="checkbox"/> SGTE	no data
<input checked="" type="checkbox"/> FToxid	<input type="checkbox"/> FSstel	<input type="checkbox"/> SGnobl	
<input type="checkbox"/> FTsalt	<input type="checkbox"/> FSups	<input type="checkbox"/> SGsold	
<input type="checkbox"/> FTmisc	<input type="checkbox"/> FSnobl	<input type="checkbox"/> SGnucl	
<input type="checkbox"/> FTall			
<input type="checkbox"/> FThelg			
<input type="checkbox"/> FTPulp		<input type="checkbox"/> TDnucl	
<input type="checkbox"/> FTlite		<input type="checkbox"/> OLIP	
		<input type="checkbox"/> OLIC	
		<input type="checkbox"/> OLIG	

Miscellaneous

EXAM SGSL SGTE*

Information

Options

Include:

gaseous ions (plasmas)
 aqueous species
 limited data compounds (25C)

Limits:

Organic species CxHy..., X(max) =
Minimum solution components: 1 2 cpts

Cancel Summary ... OK

FactSage 6.2 bet. Compound: 1/24 databases Solution: 1/22 databases

Next >

FeO-ZnO System (oxide phases only)

◀ Menu - Phase Diagram: last system

- X

File Units Parameters Variables Help

T(C) P(atm) Energy(J) Mass(mol) Vol(litre)

Components (2)

FeO + ZnO

Products

Compound species

<input type="checkbox"/> gas	<input checked="" type="radio"/> ideal	<input type="radio"/> real
<input type="checkbox"/> aqueous	0	
<input type="checkbox"/> pure liquids	0	
<input checked="" type="checkbox"/> pure solids	4	
<input checked="" type="checkbox"/> suppress duplicates <input type="button" value="apply"/>		

species: 4

Target
- none -
Estimate T(K):
Mass(mol):

Solution species

*	+	Base-Phase	Full Name
I		FToxid-SLAGA	ASlag-liq
	+	FToxid-SPINA	ASpinel
	+	FToxid-MeO_A	AMonoxide
	+	FToxid-ZNIT	Zincite

Legend
I - immiscible 1
+ - selected 3

Show all selected
species: 24
solutions: 5

Custom Solutions

0 fixed activities
0 ideal solutions
0 activity coefficients

Pseudonyms
 apply List ...

include molar volumes

Total Species (max 1500) 28
Total Solutions (max 40) 5

Variables

T(C)	ZnO/(FeO+ZnO)			
800 2000	0 1			

Phase Diagram

Y
X

FactSage 6.2 beta

FeO-ZnO System (oxide phases only)

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



Variables

Y
X

compositions

$\log_{10}(a)$

A
B C

Y steps:
X steps:

Next >>

T and P

Temperature

T(C)
 1/T(K)

Y-axis
Max:
Min:

Pressure

P(atm)
 log P

constant

Compositions (mole)

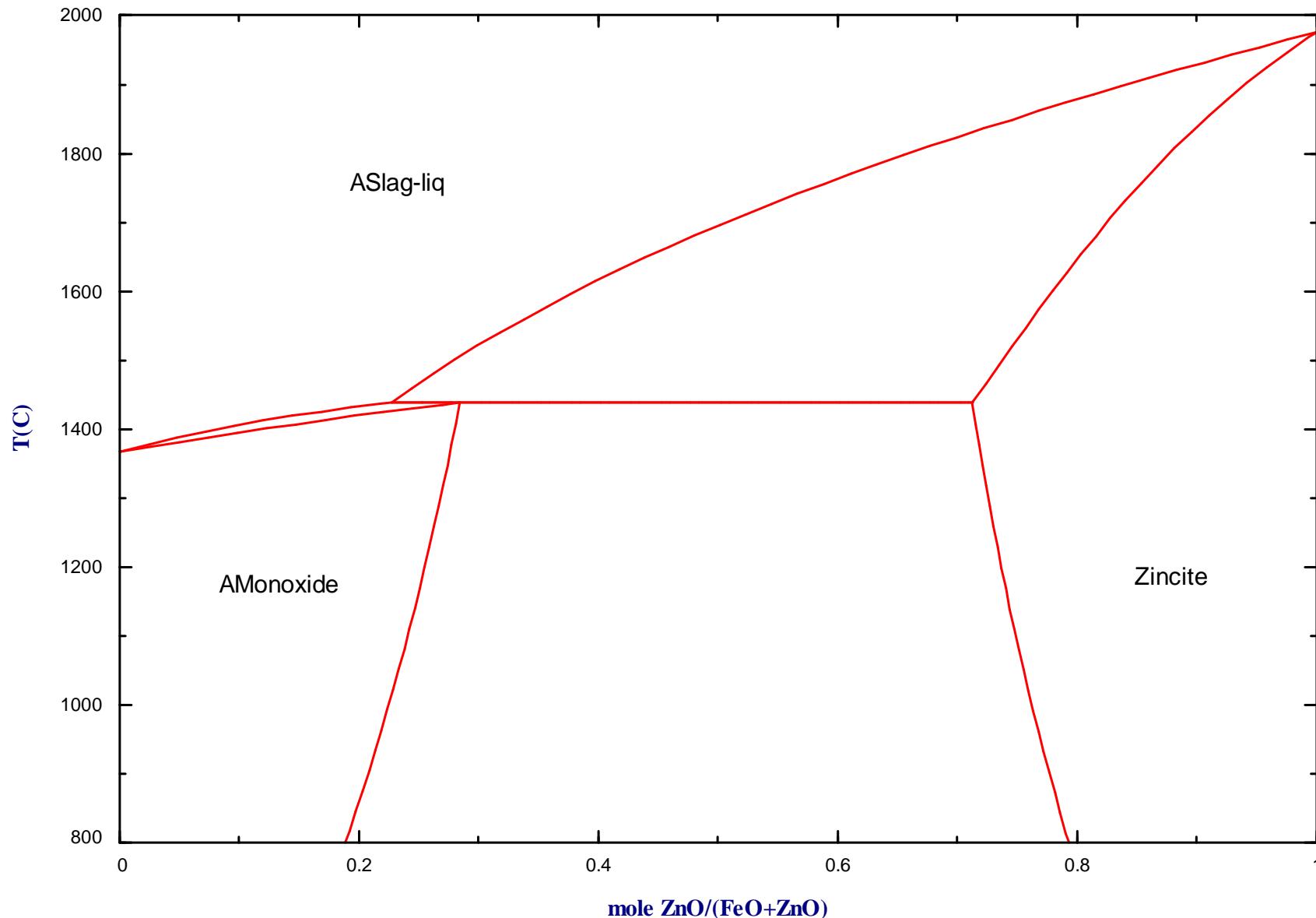
#1. $\frac{0}{1} \text{ FeO} + \frac{1}{1} \text{ ZnO} = \frac{X\text{-axis}}{1 (\text{max})}$

$\frac{1}{1} \text{ FeO} + \frac{1}{1} \text{ ZnO} = \frac{}{0 (\text{min})}$

Cancel

OK

FeO-ZnO System (oxide phases only)



FeO-ZnO System (oxide phases only)

F 1. Show Results

File Edit

1

```
T(C) = 1304, mole ZnO/(FeO+ZnO) = 0.1356
=====
FeO + ZnO =
1.0000 mol AMonoxide
(73.140 gram, 1.0000 mol)
(1304.00 C, 1 atm, a=1.0000)
( 0.86444 FeO
+ 0.13556 ZnO)

System component Mole fraction Mass fraction
FeO_wustite(s) 0.86444 0.84916
ZnO_zincite(s) 0.13556 0.15084

+ 0.00000 mol ASlag-liq#1
(1304.00 C, 1 atm, a=0.80748)
( 0.91202 FeO
+ 8.7979E-02 ZnO)

+ 0.00000 mol ASlag-liq#2
(1304.00 C, 1 atm, a=0.80748)
( 0.91202 FeO
+ 8.7979E-02 ZnO)

+ 0.00000 mol Zincite
(1304.00 C, 1 atm, a=0.68060)
( 0.43266 FeO
+ 0.56734 ZnO)
```

Phases do not have any Fe_2O_3

FeO-ZnO System (oxide phases and pure Fe)

F Menu - Phase Diagram: Metal phases are not selected

File Units Parameters Variables Help
T(C) P(atm) Energy(J) Mass(mol) Vol(litre)

Components (2)
 $\text{FeO} + \text{ZnO}$

Products

Compound species	<input type="checkbox"/> gas	<input checked="" type="radio"/> ideal	<input type="radio"/> real	0
aqueous	0			
* + pure liquids	1			
* + pure solids	6			
<input type="checkbox"/> suppress duplicates	<input type="button" value="apply"/>			
* - custom selection	species: 7			

Solution species

*	+	Base-Phase	Full Name
	I	FToxid-SLAGA	ASlag-liq
	+	FToxid-SPINA	ASpinel
	+	FToxid-MeO_A	AMonoxide
	+	FToxid-ZNIT	Zincite

Target
- none -
Estimate T(K): 1000
Mass(mol): 0

Legend
I - immiscible 1
+ - selected 3
 Show all selected
species: 24
solutions: 5

Variables

T(C)	ZnO/(FeO+ZnO)			
800 2000	0 1			

T(C) vs ZnO/(FeO+ZnO)

FactSage 6.2 beta | g:\...\PhasFe-Zn-O_FeO-ZnO_no-Fe2O3.DAT

F Selection - Equilib

Selected: 6/17 Duplicates selected. SOLID Sorted by Code

+	Code	Species	Data	Phase	T	V	Activity
+	13	Fe(s)	FACT53	bcc			
+	14	Fe(s2)	FACT53	fcc			
	15	FeO(s)	FACT53	wustite	V		
	16	Fe2O3(s)	FACT53	hematite	V		
	17	Fe2O3(s2)	FACT53	high-pressure-...	V		
	18	Fe2O3(s3)	FACT53	high-pressure-...	V		
	19	Fe3O4(s)	FACT53	magnetite	V		
	20	Fe3O4(s2)	FACT53	magnetite	V		
	21	Fe3O4(s3)	FACT53	high-pressure-...	V		
	22	Fe3O4(s4)	FACT53	high-pressure-...	V		
	23	Zn(s)	FACT53	solid			
	24	ZnO(s)	FACT53	zincite			
	25	ZnFe2O4(s)	FACT53	solid			
+	26	Fe2O3(s)	FToxid	hematite	V		
+	27	Fe2O3(s2)	FToxid	high-pressure-...	V		
+	28	Fe2O3(s3)	FToxid	high-pressure-...	V		
+	29	ZnO(s)	FToxid	zincite			

F Selection - Equilib

Selected: 1/6 Duplicates selected. LIQUID Sorted by Code

+	Code	Species	Data	Phase	T	V	Activity
+	7	Fe(liq)	FACT53	liquid			
	8	FeO(liq)	FACT53	liquid			
	9	Fe3O4(liq)	FACT53	liquid			
	10	Zn(liq)	FACT53	liquid			
	11	ZnO(liq)	FACT53	liquid			
	12	ZnO(liq)	FToxid	liquid			

FeO-ZnO System (oxide phases and pure Fe)

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



Variables

Y
X

compositions

$\log_{10}(a)$

A
B C

Y steps:
X steps:

Next >>

T and P

Temperature

T(C)
 1/T(K)

Y-axis
Max:
Min:

Pressure

P(atm)
 log P

constant

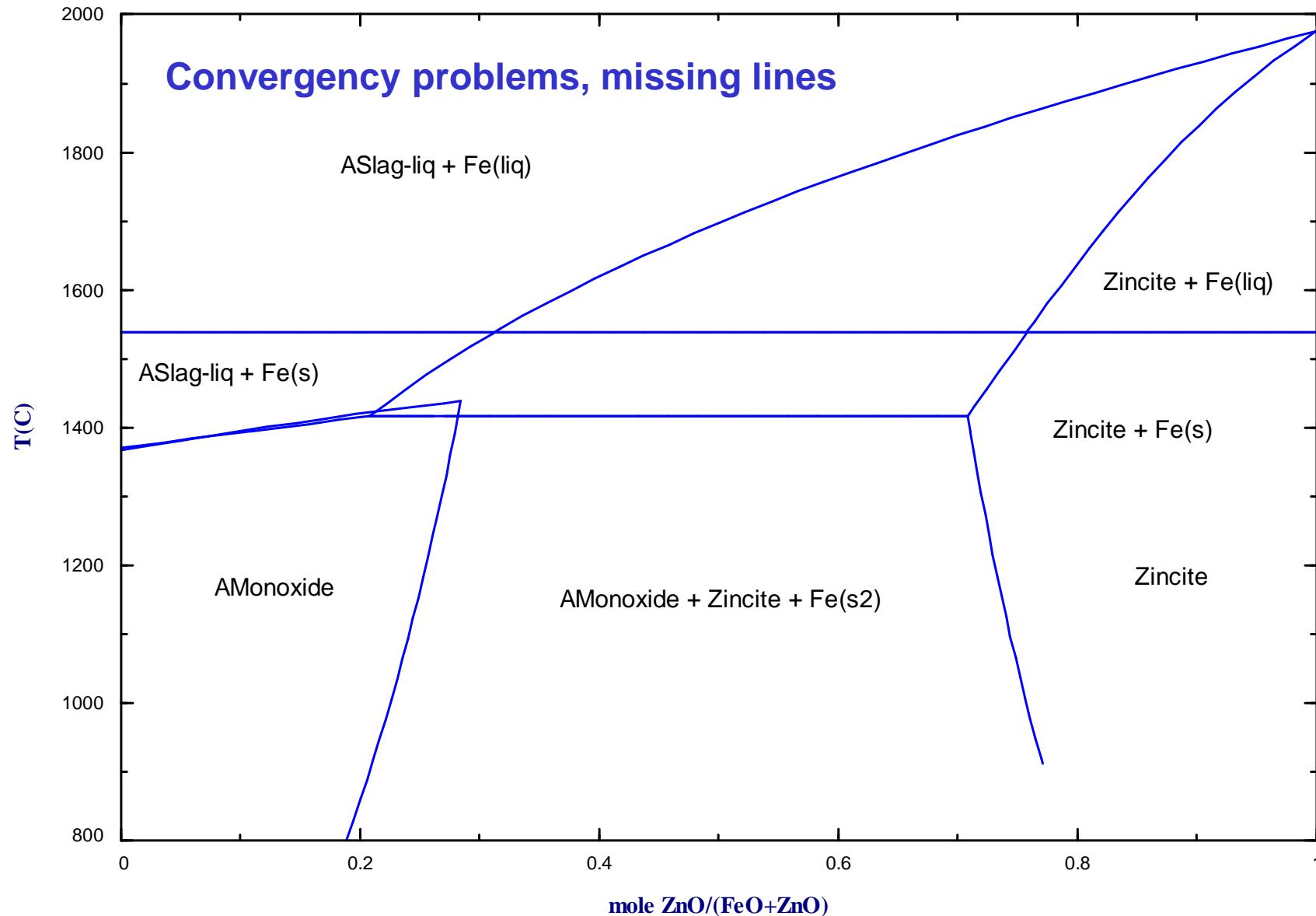
Compositions (mole)

#1. $\frac{0}{1} \text{ FeO} + \frac{1}{1} \text{ ZnO} = \frac{X\text{-axis}}{1 \text{ (max)}} \text{ } \frac{0 \text{ (min)}}{\text{ }}$

Cancel

OK

FeO-ZnO System (oxide phases and pure Fe)



FeO-ZnO System in Equilibrium with Metals

F Components - Phase Diagram

File Edit Units Data Search Help

T(C) P(atm) Energy(J) Mass(mol) Vol(litre)

Components

FeO
ZnO
Fe

1 - 3

Data Search

Databases - 2/24 compound databases, 2/22 solution databases

Fact **FactSage™ SGTE**

<input type="checkbox"/> ELEM	<input type="checkbox"/> FSopp	<input type="checkbox"/> BINS	compounds only
<input type="checkbox"/> FACT	<input type="checkbox"/> FSlead	<input type="checkbox"/> SGPS	solutions only
<input type="checkbox"/> Fact53	<input type="checkbox"/> FSlite	<input type="checkbox"/> SGTE	no data
<input checked="" type="checkbox"/> FToxid	<input checked="" type="checkbox"/> FSstel	<input type="checkbox"/> SGnobl	<input type="checkbox"/> Clear All
<input type="checkbox"/> FTsalt	<input type="checkbox"/> FSups	<input type="checkbox"/> SGsold	<input type="checkbox"/> Select All
<input type="checkbox"/> FTmisc	<input type="checkbox"/> FSnobl	<input type="checkbox"/> SGnucl	<input type="checkbox"/> Add/Remove Data
<input type="checkbox"/> FThall			<input type="checkbox"/> RefreshDatabases
<input type="checkbox"/> FThelg			
<input type="checkbox"/> FTpulp			
<input type="checkbox"/> FTlite			

Miscellaneous

EXAM SGSL SGTE*

Other

<input type="checkbox"/> TDnucl	<input type="checkbox"/> OLIP	<input type="checkbox"/> OLIC	<input type="checkbox"/> OLIL
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Information

Oxide phases

Metal phases from FSstel

Options

Default

Include

gaseous ions (plasmas)
 aqueous species
 limited data compounds (25C)

Limits

Organic species CxHy..., X(max) =
Minimum solution components: 1 2 cpts

Cancel Summary ... OK

FactSage 6.2 bet. Compound: 2/24 databases Solution: 2/22 databases

Next >

FeO-ZnO System in Equilibrium with Metals

F Menu - Phase Diagram: Correct phase diagram Fe...

File Units Parameters Variables Help

T(C) P(atm) Energy(J) Mass(mol) Vol(litre)

Components (3) FeO + ZnO + Fe

Products

Compound species	gas <input checked="" type="radio"/> ideal <input type="radio"/> real	0
aqueous	<input type="checkbox"/>	0
pure liquids	<input type="checkbox"/>	0
* pure solids	<input checked="" type="checkbox"/>	7
<input type="checkbox"/> suppress duplicates	<input type="button" value="apply"/>	
* - custom selection		
species:	7	

Solution species

*	+	Base-Phase	Full Name
	+	FSstel-FEZ1	FEZN4
	+	FSstel-FEZ2	FEZN_DELTA
	+	FSstel-FEZ3	FEZN_ZETA
	+	FSstel-HCP	HCP_A3:Me2(C,N)
I		FToxid-SLAGA	ASlag-liq
	+	FToxid-SPINA	ASpinel
	+	FToxid-MeO_A	AMonoxide
	+	FToxid-ZNIT	Zincite

Custom Solutions

- fixed activities
- ideal solutions
- activity coefficients

Details ...

Target

- none -

Estimate T(K):

Mass(mol):

Legend

- I - immiscible 1
- + - selected 12

Show all selected

species: 51
solutions: 14

Variables

T(C)	ZnO/(FeO+ZnO+)	Fe/(FeO+ZnO+Fe)		
800 2000	0 1	0.001		

FactSage 6.2 beta g:\...\PhasFe-Zn-O_FeO-ZnO-Fe_using-FSstel.DAT

F Selection - Equilib

File Edit Show Sort

Selected: 7/10 Duplicates selected: SOLID Sorted by Code

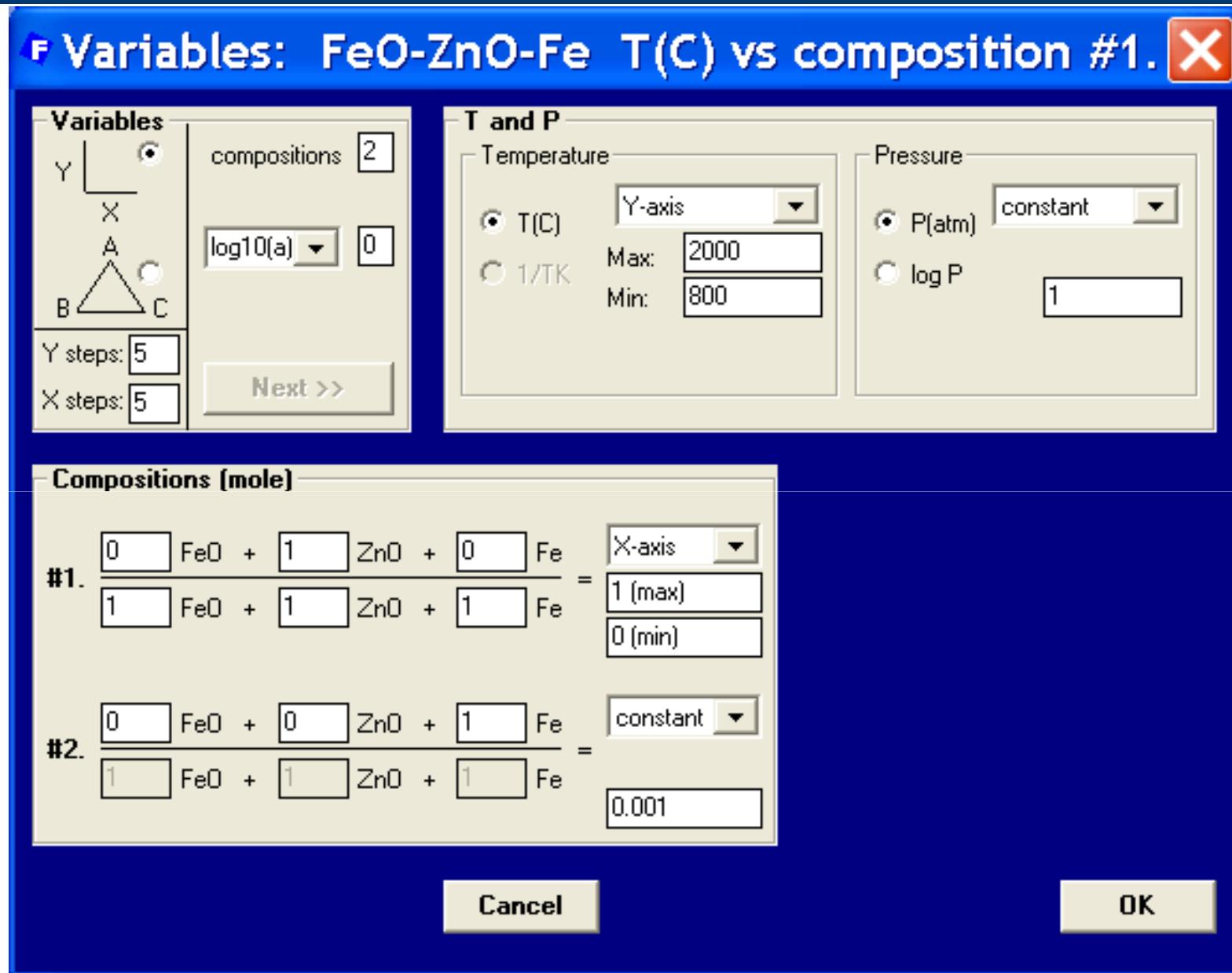
+	Code	Species	Data	Phase	T	V	Activity
+	5	Fe(s)	FSstel	bcc_a2			
+	6	Fe(s2)	FSstel	fcc_a1			
	7	Fe2O3(s)	FSstel	hematite		V	
	8	Fe3O4(s)	FSstel	magnetite		V	
	9	Fe3O4(s2)	FSstel	magnetite		V	
+	10	Zn(s)	FSstel	hcp_zn	o		
+	11	Fe2O3(s)	FToxid	hematite		V	
+	12	Fe2O3(s2)	FToxid	high-pressure...		V	
+	13	Fe2O3(s3)	FToxid	high-pressure...		V	
+	14	ZnO(s)	FToxid	zincite			

Oxide phases

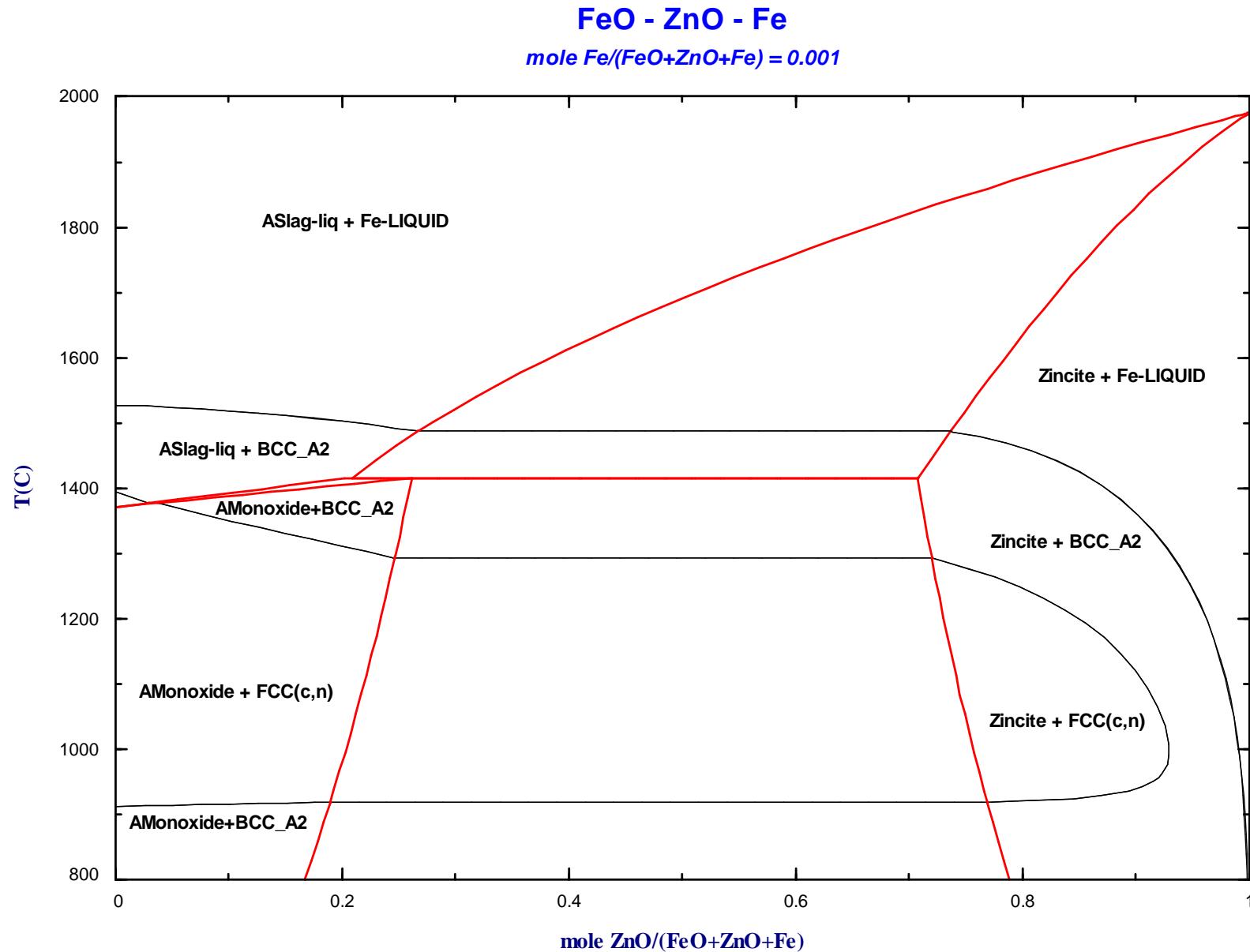
Metal phases from FSstel

Show Selected Select All Select/Clear... Clear OK

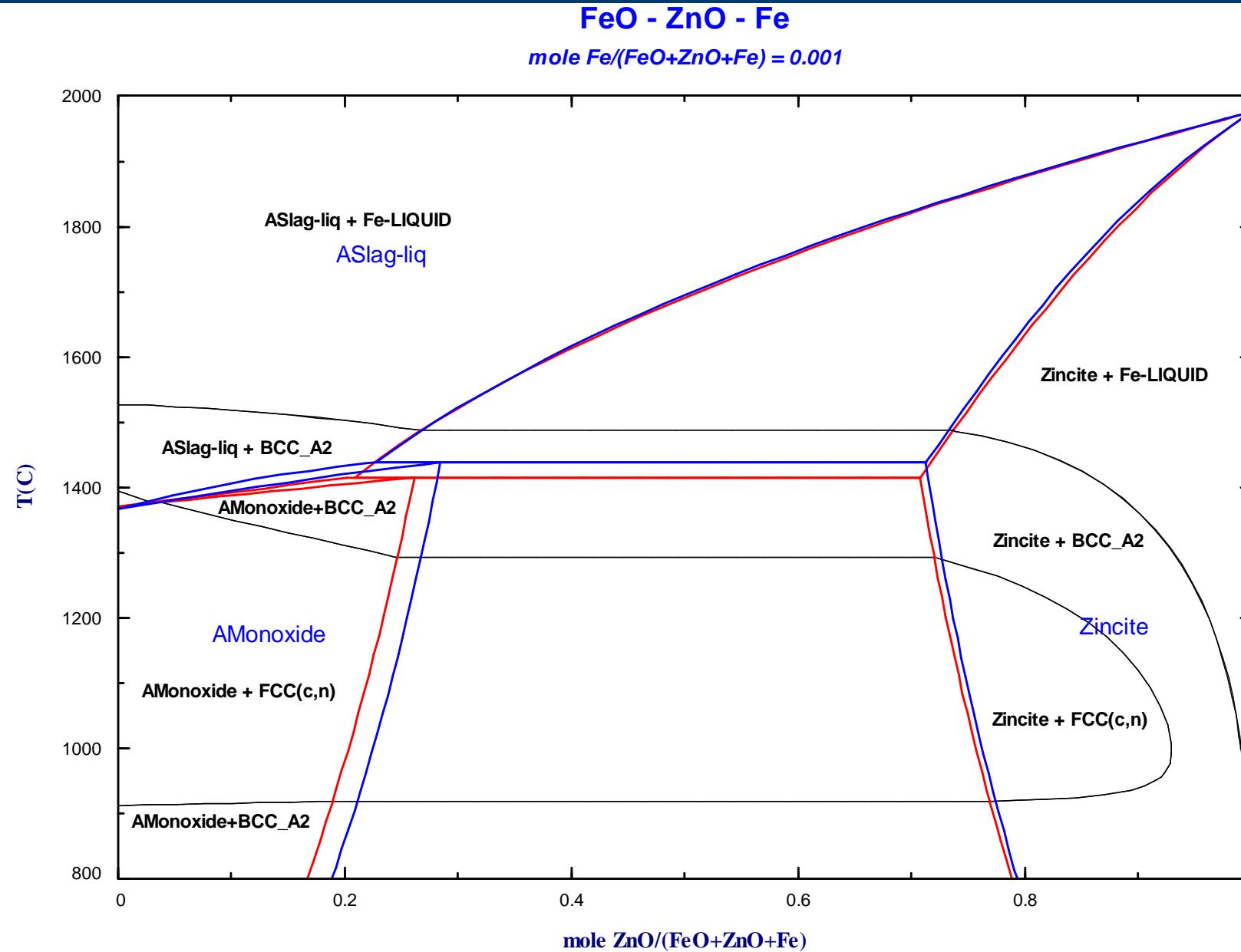
FeO-ZnO System in Equilibrium with Metals



FeO-ZnO System in Equilibrium with Metals



FeO-ZnO in Equilibrium with Metals vs FeO-ZnO



FeO-ZnO System in Equilibrium with Metals

Data Search

Databases - 2/24 compound databases, 2/22 solution databases

Fact **FactSage™** **SGTE**

<input type="checkbox"/> ELEM	<input type="checkbox"/> FScopp	<input type="checkbox"/> BINS	<input type="checkbox"/> compounds only
<input type="checkbox"/> FACT	<input type="checkbox"/> FSlead	<input type="checkbox"/> SGPS	<input type="checkbox"/> solutions only
<input type="checkbox"/> Fact53	<input type="checkbox"/> FSlite	<input checked="" type="checkbox"/> SGTE	<input type="checkbox"/> no data
<input checked="" type="checkbox"/> FToxid	<input type="checkbox"/> FSstel	<input type="checkbox"/> SGnobl	
<input type="checkbox"/> FTsalt	<input type="checkbox"/> FSups	<input type="checkbox"/> SGsold	
<input type="checkbox"/> FTmisc	<input type="checkbox"/> FSnobl	<input type="checkbox"/> SGnucl	
<input type="checkbox"/> FThall			
<input type="checkbox"/> FThelg			
<input type="checkbox"/> FTpulp	Other	<input type="checkbox"/> TDnucl	
<input type="checkbox"/> FTlite	<input type="checkbox"/> OLIP	<input type="checkbox"/> OLIC	
	<input type="checkbox"/> OLIG	<input type="checkbox"/> OLIL	

Miscellaneous

EXAM SGSL SGTE*

Information -

Oxide phases

Metal phases from SGTE

Options

Include:

gaseous ions (plasmas)
 aqueous species
 limited data compounds (25C)

Limits:

Organic species CxHy..., X(max) =
Minimum solution components: 1 2 cpts

FeO-ZnO System in Equilibrium with Metals

F Menu - Phase Diagram: Correct phase diagram Fe...

File Units Parameters Variables Help

T(C) P(atm) Energy(J) Mass(mol) Vol(litre)

Components (3)

FeO + ZnO + Fe

Products

Compound species	0
gas	ideal
aqueous	0
pure liquids	0
pure solids	7
suppress duplicates	<input type="checkbox"/> apply
species:	7

Solution species

*	+	Base-Phase	Full Name
I	FToxid-SLAGA	ASlag-liq	
+	FToxid-SPINA	ASpinel	
+	FToxid-MeO_A	AMonoxide	
+	FToxid-ZNIT	Zincite	
+	SGTE-LIQU	LIQUID	
+	SGTE-FCC1	FCC_A1	
+	SGTE-BCC1	BCC_A2	
+	SGTE-HCP1	HCP_A3	

Target
- none -
Estimate T(K): 1000
Mass(mol): 0

Legend
I - immiscible 1
+ - selected 11

Show all selected
species: 51
solutions: 13

Variables

T(C)	ZnO/(FeO+ZnO+)	Fe/(FeO+ZnO+Fe)		
800 2000	0 1	0.001		

Phase Diagram

Y X Calculate >>

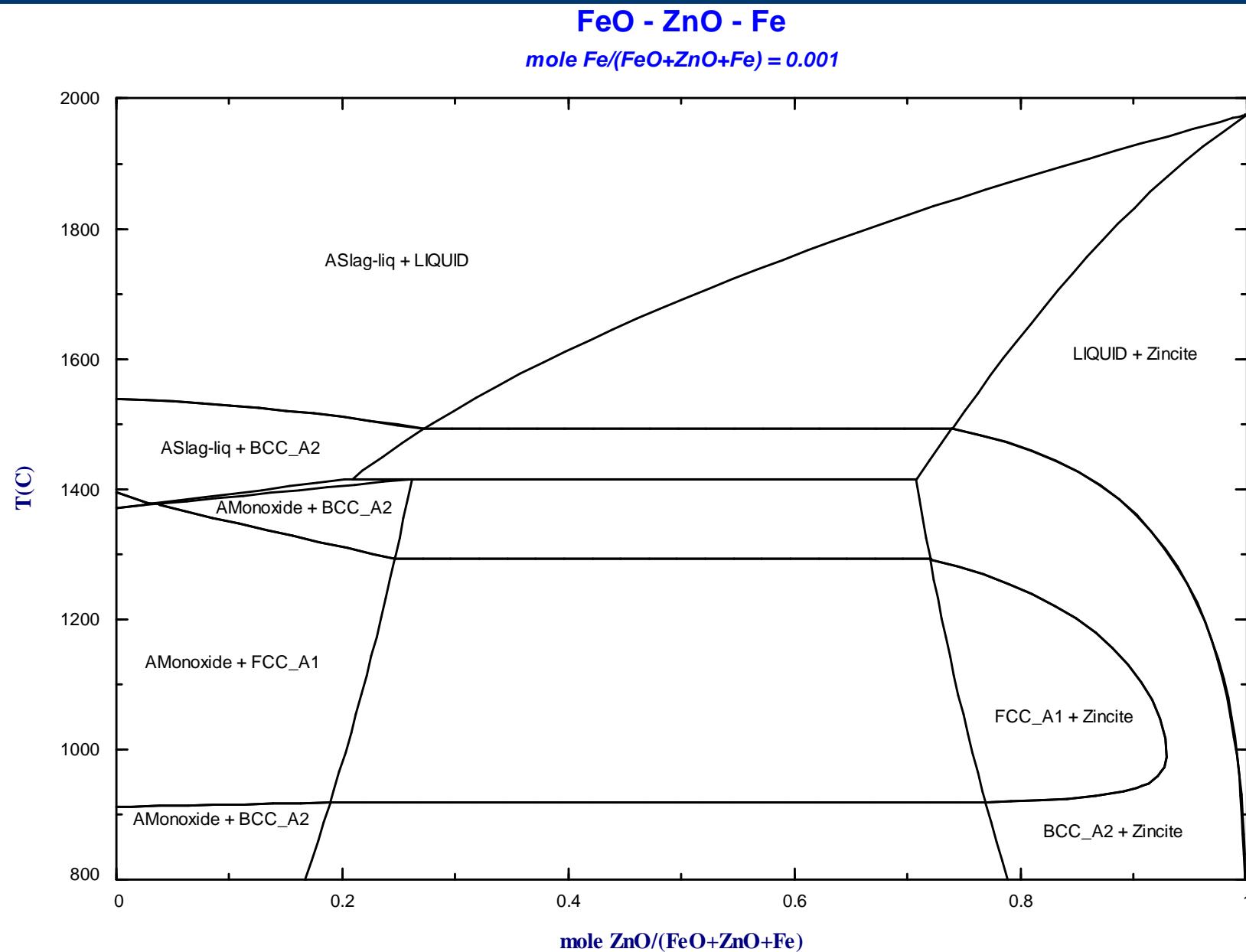
FactSage 6.2 beta g:\...\PhasFe-Zn-O_FeO-ZnO-Fe_SGTE.DAT

F Selection - Equilib

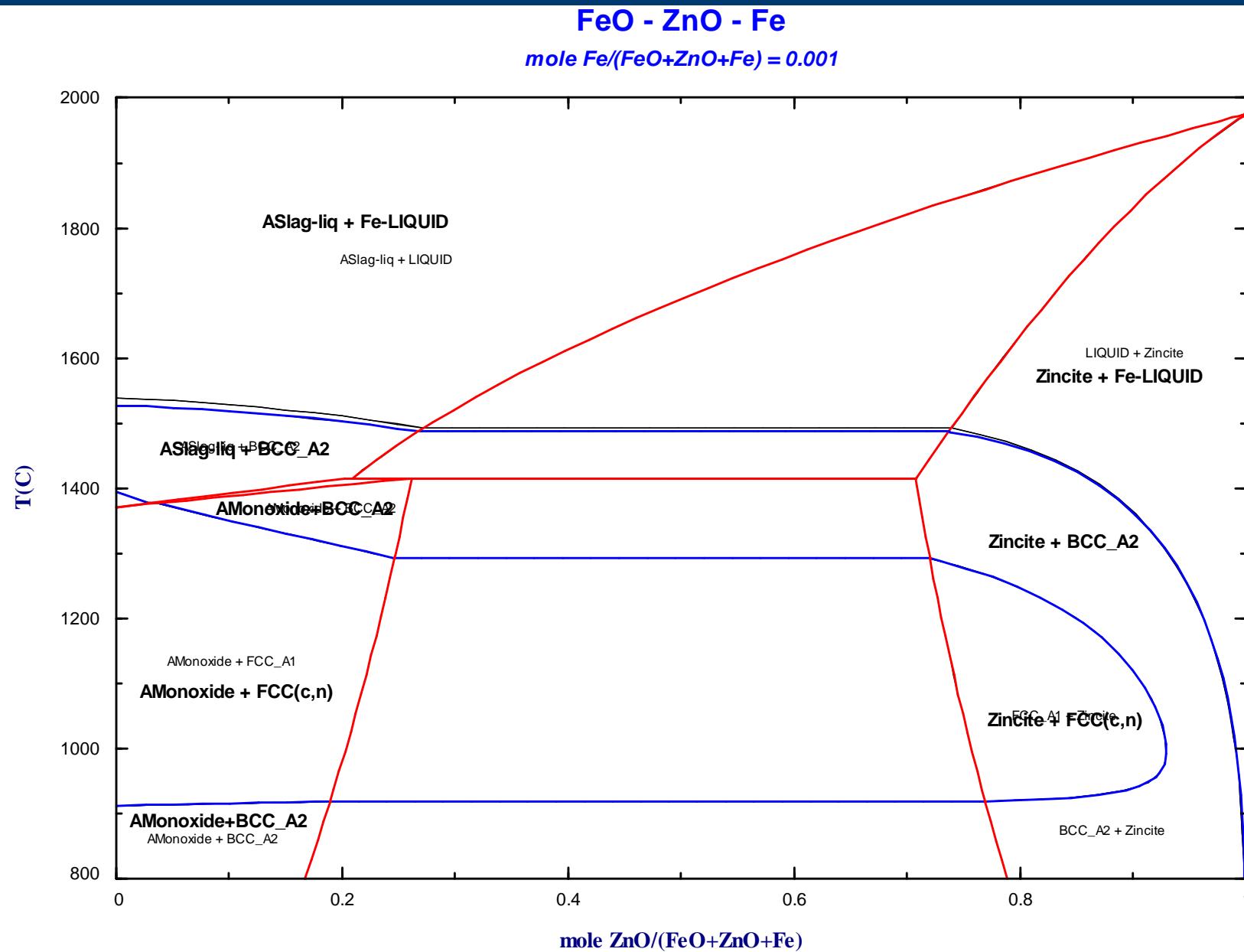
Oxide phases

Metal phases from SGTE

FeO-ZnO System in Equilibrium with Metals



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



FeO-ZnO System in Equilibrium with Metals

Data Search

Databases - 2/24 compound databases, 1/22 solution databases

Fact **FactSage™** **SGTE**

<input type="checkbox"/> ELEM	<input type="checkbox"/> FScopp	<input type="checkbox"/> BINS	<input type="checkbox"/> compounds only
<input type="checkbox"/> FACT	<input type="checkbox"/> FSlead	<input type="checkbox"/> SGPS	<input type="checkbox"/> solutions only
<input checked="" type="checkbox"/> Fact53	<input type="checkbox"/> FSlite	<input type="checkbox"/> SGTE	<input type="checkbox"/> no data
<input checked="" type="checkbox"/> FToxid	<input type="checkbox"/> FSstel	<input type="checkbox"/> SGnobl	
<input type="checkbox"/> FTsalt	<input type="checkbox"/> FSups	<input type="checkbox"/> SGsold	
<input type="checkbox"/> FTmisc	<input type="checkbox"/> FSnobl	<input type="checkbox"/> SGnucl	
<input type="checkbox"/> FThall			
<input type="checkbox"/> FTholg			
<input type="checkbox"/> FTpulp			
<input type="checkbox"/> FTlite			

Miscellaneous

<input type="checkbox"/> EXAM	<input type="checkbox"/> SGSL	<input type="checkbox"/> SGTE*
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Other

<input type="checkbox"/> TDnucl	<input type="checkbox"/> OLIC	<input type="checkbox"/> OLIL
<input type="checkbox"/> OLIP	<input type="checkbox"/> OLIG	
<input type="checkbox"/> OLIG		

Clear All Select All Add/Remove Data RefreshDatabases

Information -

Oxide phases

Stoichiometric metal phases from Fact53

Options

Include:

<input type="checkbox"/> gaseous ions (plasmas)
<input checked="" type="checkbox"/> aqueous species
<input checked="" type="checkbox"/> limited data compounds (25C)

Limits:

Organic species CxHy..., X(max) = <input type="text" value="2"/>
Minimum solution components: <input type="radio"/> 1 <input checked="" type="radio"/> 2 cpts

Cancel Summary ... OK

FeO-ZnO System in Equilibrium with Metals

F Menu - Phase Diagram: FeO-ZnO in equilibrium wi...

File Units Parameters Variables Help

T(C) P(atm) Energy(J) Mass(mol) Vol(litre)

Components (3)

FeO + ZnO + Fe

Products

Compound species

- gas ideal real 0
- aqueous 0
- * pure liquids 1
- * pure solids 6
- suppress duplicates
- * - custom selection species: 7

Solution species

*	+	Base-Phase	Full Name
*	+	FToxid-SLAGA	ASlag-liq
	+	FToxid-SPINA	ASpinel
	+	FToxid-MeO_A	AMonoxide
	+	FToxid-ZNIT	Zincite

Custom Solutions

- 0 fixed activities
- 0 ideal solutions
- 0 activity coefficients

Pseudonyms

apply List

include molar v

Target
- none -
Estimate T(K): 1000
Mass(mol): 0

Legend
I - immiscible 1
+ - selected 3

Show all selected
species: 24
solutions: 5

Variables

T(C)	ZnO/(FeO+ZnO+Fe)	Fe/(FeO+ZnO+Fe)		
800 2000	0 1	0.001		

T(C) vs ZnO/(FeO+ZnO+Fe)

FactSage 6.2 beta g:\...\PhasFe-Zn-O_FeO-ZnO-Fe_Fe(S-L).DAT

F Selection - Equilib

File Edit Show Sort

Selected: 6/17 Duplicates selected. SOLID Sorted by Code

+	Code	Species	Data	Phase	T	V	Activity
+	13	Fe(s)	FACT53	bcc			
+	14	Fe(s2)	FACT53	fcc			
	15	FeO(s)	FACT53	wustite	V		
	16	Fe2O3(s)	FACT53	hematite	V		
	17	Fe2O3(s2)	FACT53	high-pressure...	V		
	18	Fe2O3(s3)	FACT53	high-pressure...	V		
	19	Fe3O4(s)	FACT53	magnetite	V		
	20	Fe3O4(s2)	FACT53	magnetite	V		
	21	Fe3O4(s3)	FACT53	high-pressure...	V		
	22	Fe3O4(s4)	FACT53	high-pressure...	V		
	23	Zn(s)	FACT53	solid			
	24	ZnO(s)	FACT53	zincite			
	25	ZnFe2O4(s)	FACT53	solid			
+	26	Fe2O3(s)	FToxid	hematite	V		
+	27	Fe2O3(s2)	FToxid	high-pressure...	V		
+	28	Fe2O3(s3)	FToxid	high-pressure...	V		
+	29	ZnO(s)	FToxid	zincite			

F Selection - Equilib

File Edit Show Sort

Selected: 1/6 Duplicates selected. LIQUID Sorted by Code

+	Code	Species	Data	Phase	T	V	Activity
+	7	Fe(liq)	FACT53	liquid			
	8	FeO(liq)	FACT53	liquid			
	9	Fe3O4(liq)	FACT53	liquid			
	10	Zn(liq)	FACT53	liquid			
	11	ZnO(liq)	FACT53	liquid			
	12	ZnO(liq)	FToxid	liquid			

Show Selected Select All Select/Clear... Clear OK

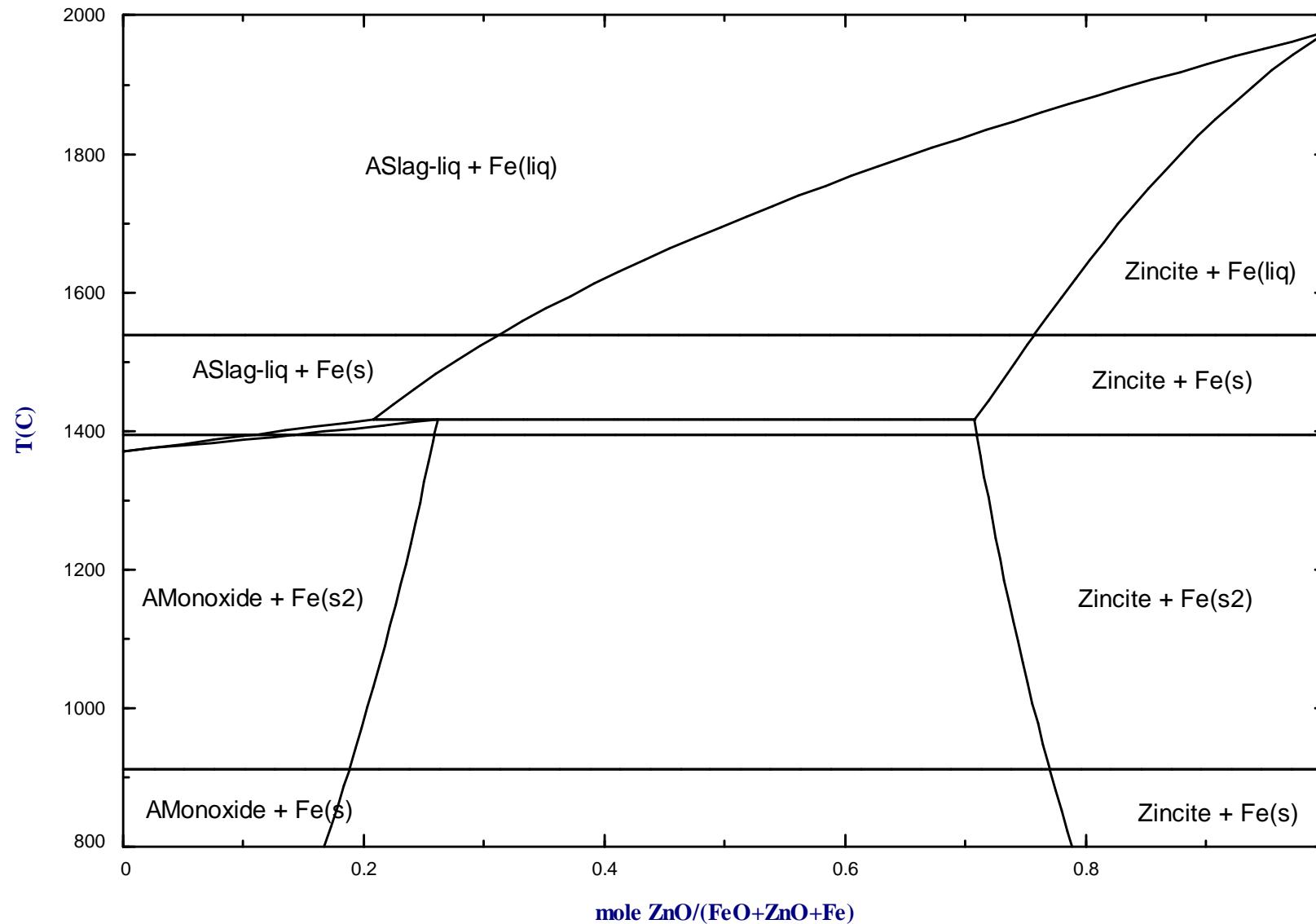
Oxide phases

Stoichiometric metal phases from Fact53

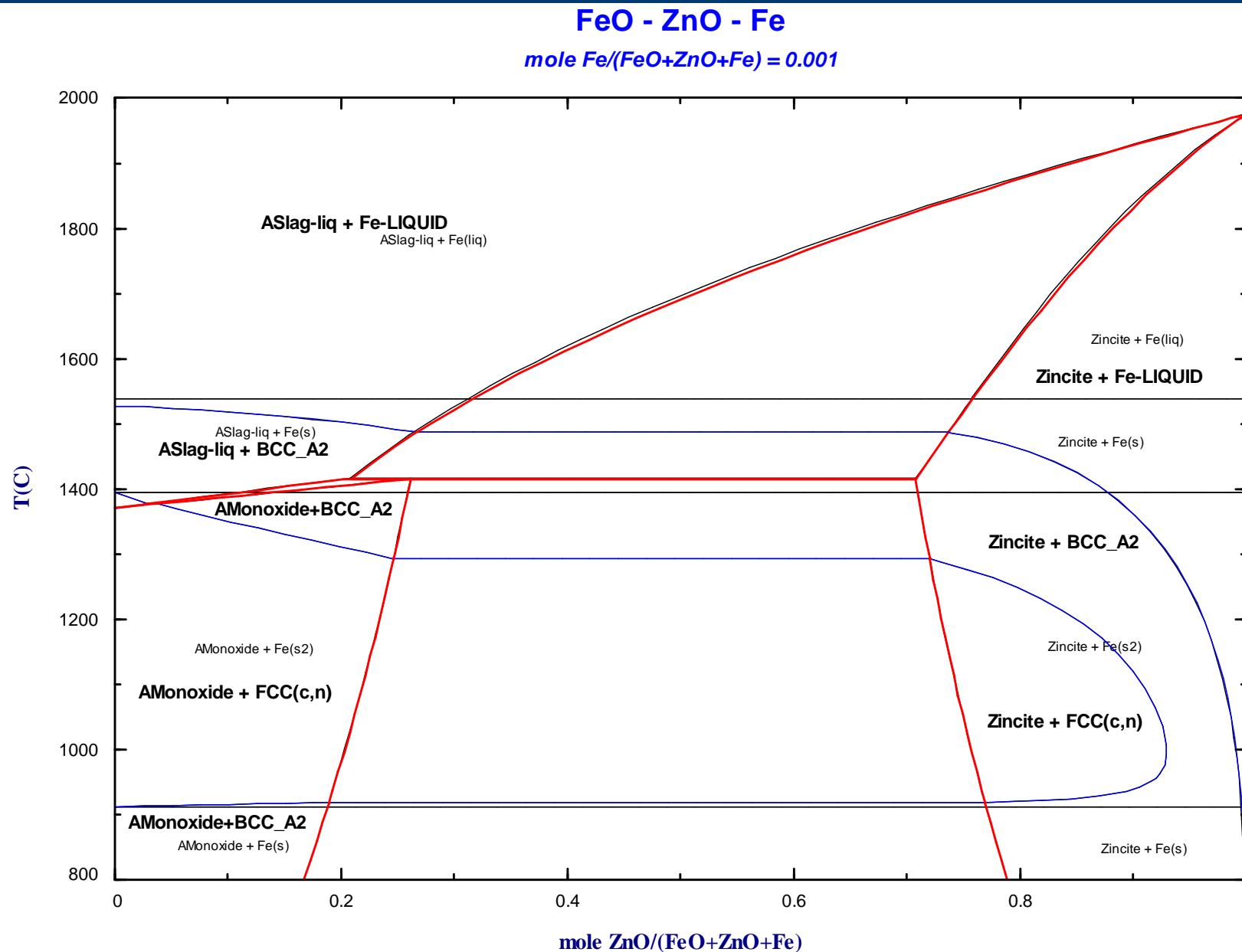
FeO-ZnO System in Equilibrium with Metals

FeO - ZnO - Fe

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



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



FeO-ZnO System in Equilibrium with Metals

Menu - Phase Diagram: FeO-ZnO in equilibrium wi...

File Units Parameters Variables Help

T(C) P(atm) Energy(J) Mass(mol) Vol(litre)

Components (3)

FeO + ZnO + Fe

Products

Compound species			
gas	<input checked="" type="radio"/> ideal	<input type="radio"/> real	0
aqueous			0
pure liquids			0
* pure solids			5
<input type="checkbox"/> suppress duplicates	<input type="button" value="apply"/>		
* - custom selection			species: 5

Solution species

*	+	Base-Phase	Full Name
	I	FToxid-SLAGA	ASlag-liq
	+	FToxid-SPINA	ASpinel
	+	FToxid-MeO_A	AMonoxide
	+	FToxid-ZNIT	Zincite

Target
- none -
Estimate T(K): 1000
Mass(mol): 0

Variables

T(C)	ZnO/(FeO+ZnO+Fe)	Fe/(FeO+ZnO+Fe)		
800 2000	0 1	0.001		

T(C) vs ZnO/(FeO+ZnO+Fe)

FactSage 6.2 beta g:\...\PhasFe-Zn-O_FeO-ZnO-Fe_Fe(S-L).DAT

Oxide phases

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

Selection - Equilib

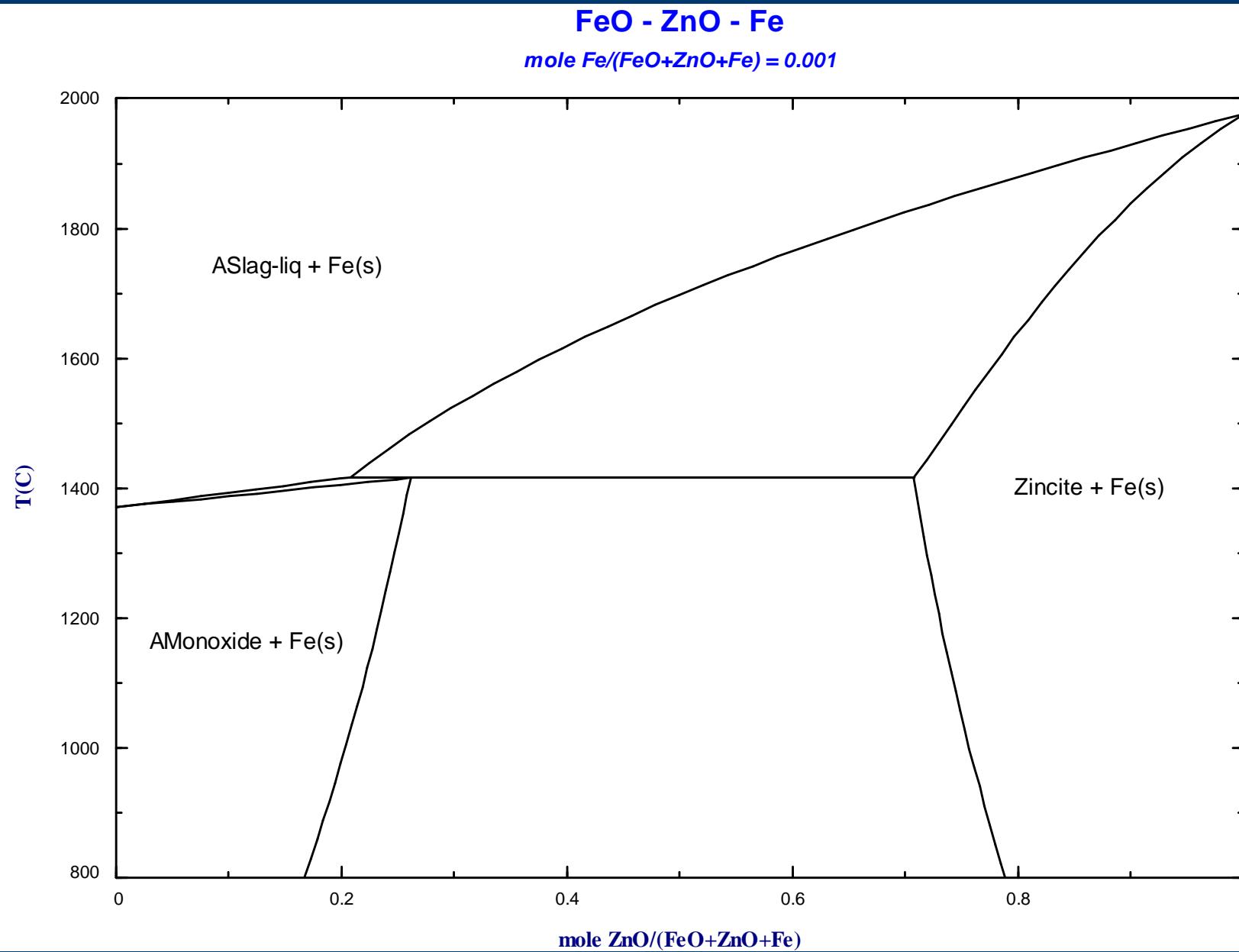
File Edit Show Sort

Selected: 5/17 Duplicates selected. SOLID Sorted by Code

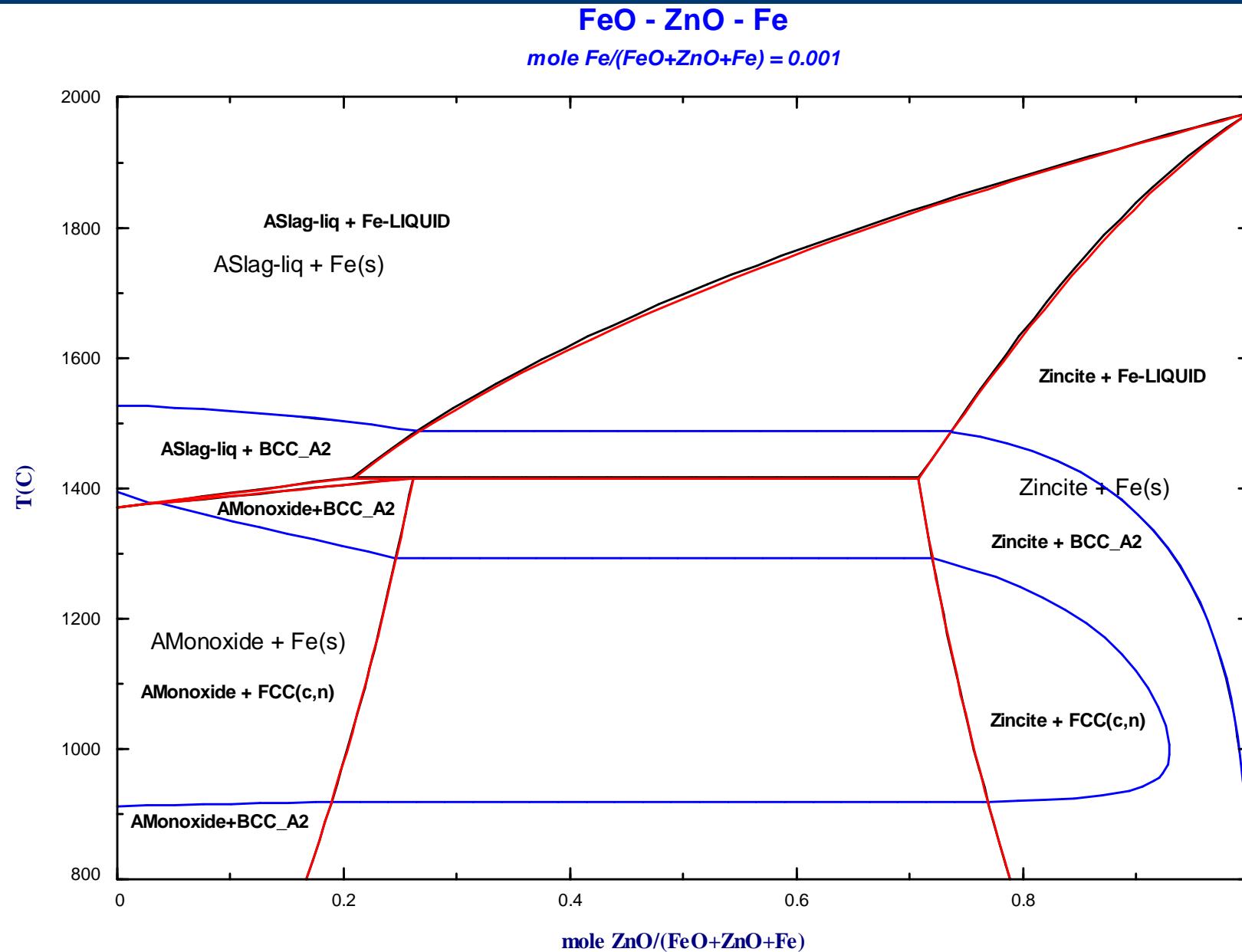
+	Code	Species	Data	Phase	T	V	Activity
+	13	Fe(s)	FACT53	bcc			
+	14	Fe(s2)	FACT53	fcc			
+	15	FeO(s)	FACT53	wustite	V		
	16	Fe2O3(s)	FACT53	hematite	V		
	17	Fe2O3(s2)	FACT53	high-pressure...	V		
	18	Fe2O3(s3)	FACT53	high-pressure...	V		
	19	Fe3O4(s)	FACT53	magnetite	V		
	20	Fe3O4(s2)	FACT53	magnetite	V		
	21	Fe3O4(s3)	FACT53	high-pressure...	V		
	22	Fe3O4(s4)	FACT53	high-pressure...	V		
	23	Zn(s)	FACT53	solid			
	24	ZnO(s)	FACT53	zincite			
	25	ZnFe2O4(s)	FACT53	solid			
+	26	Fe2O3(s)	FToxid	hematite	V		
+	27	Fe2O3(s2)	FToxid	high-pressure...	V		
+	28	Fe2O3(s3)	FToxid	high-pressure...	V		
+	29	ZnO(s)	FToxid	zincite			

Show Selected Select All Select/Clear... Clear OK

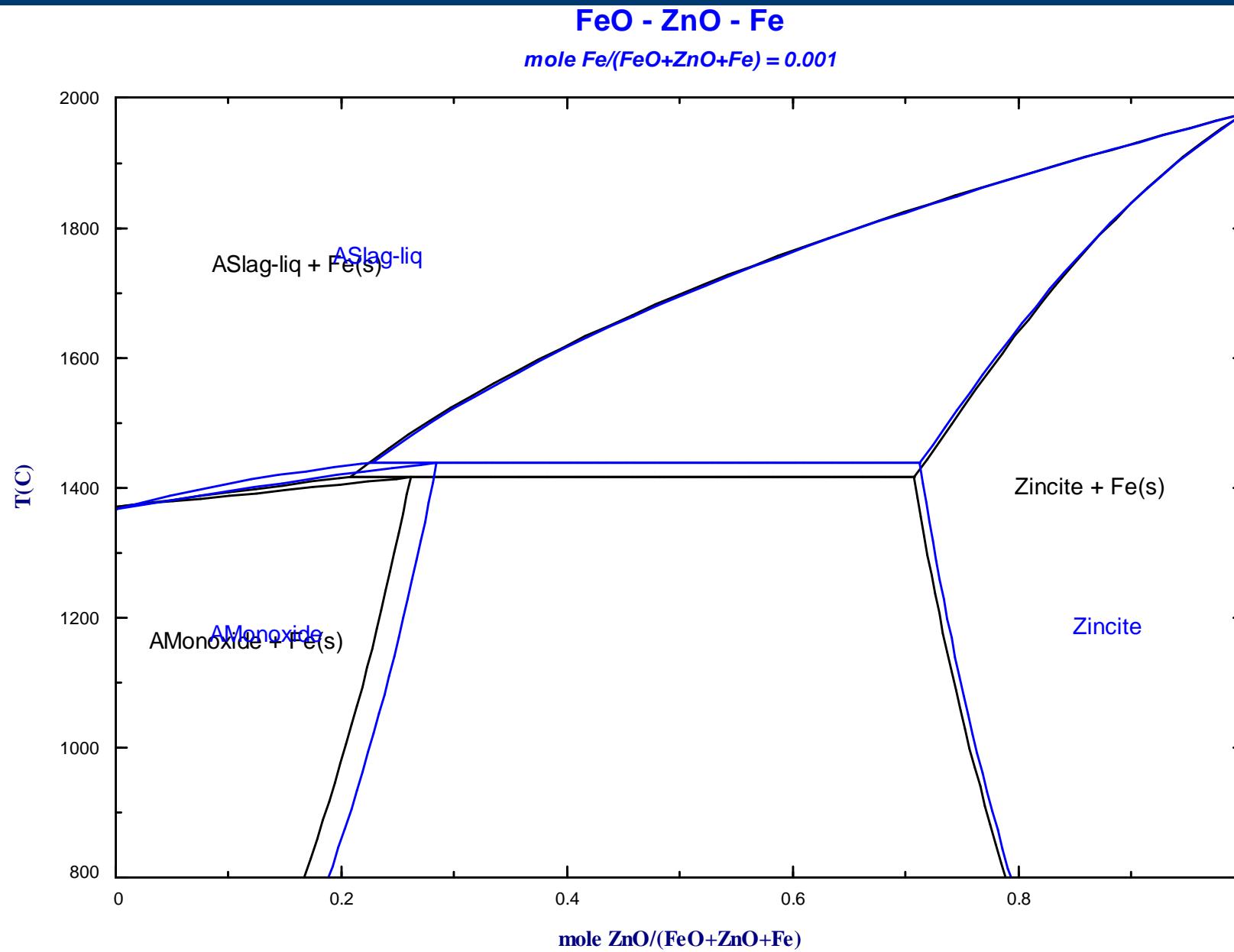
FeO-ZnO System in Equilibrium with Metals



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



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



FeO-ZnO System in Equilibrium with Metals

Menu - Phase Diagram: FeO-ZnO in equilibrium

File Units Parameters Variables Help

T(C) P(atm) Energy(J) Mass(mol) Vol(litre)

Components (3)

FeO + ZnO + Fe

Products

Compound species	
gas	<input checked="" type="radio"/> ideal <input type="radio"/> real
aqueous	0
* pure liquids	2
* pure solids	7
suppress duplicates	<input type="checkbox"/> apply
* - custom selection	
species:	9

Solution species

*	+	Base-Phase	Full Name
	I	FToxid-SLAGA	ASlag-liq
*	+	FToxid-SPINA	ASpinel
*	+	FToxid-MeO_A	AMonoxide
	+	FToxid-ZNIT	Zincite

Legend
I - immiscible 1
+ - selected 3

Show all selected
species: 24
solutions: 5

Target
- none -
Estimate T(K): 1000
Mass(mol): 0

Variables

T(C)	ZnO/(FeO+ZnO+Fe)	Fe/(FeO+ZnO+Fe)		
800 2000	0 1	0.001		

T(C) vs ZnO/(FeO+ZnO+Fe)

FactSage 6.2 beta g:\...\PhasFe-Zn-O_FeO-ZnO-Fe_Fe(S-L).DAT

Selection - Equilib

Selected: 7/17 Duplicates selected. SOLID Sorted by Code

+	Code	Species	Data	Phase	T	V	Activity
+	13	Fe(s)	FACT53	bcc			
+	14	Fe(s2)	FACT53	fcc			
	15	FeO(s)	FACT53	wustite	V		
	16	Fe2O3(s)	FACT53	hematite	V		
	17	Fe2O3(s2)	FACT53	high-pressure	V		
	18	Fe2O3(s3)	FACT53	high-pressure	V		
	19	Fe3O4(s)	FACT53	magnetite	V		
	20	Fe3O4(s2)	FACT53	magnetite	V		
	21	Fe3O4(s3)	FACT53	high-pressure	V		
	22	Fe3O4(s4)	FACT53	high-pressure	V		
+	23	Zn(s)	FACT53	solid			
	24	ZnO(s)	FACT53	zincite			
	25	ZnFe2O4(s)	FACT53	solid			
+	26	Fe2O3(s)	FToxid	hematite	V		
+	27	Fe2O3(s2)	FToxid	high-pressure	V		
+	28	Fe2O3(s3)	FToxid	high-pressure	V		
+	29	ZnO(s)	FToxid	zincite			

Selection - Equilib

Selected: 2/6 Duplicates selected. LIQUID Sorted by Code

+	Code	Species	Data	Phase	T	V	Activity
+	7	Fe(liq)	FACT53	liquid			
	8	FeO(liq)	FACT53	liquid			
	9	Fe3O4(liq)	FACT53	liquid			
+	10	Zn(liq)	FACT53	liquid			
	11	ZnO(liq)	FACT53	liquid			
	12	ZnO(liq)	FToxid	liquid			

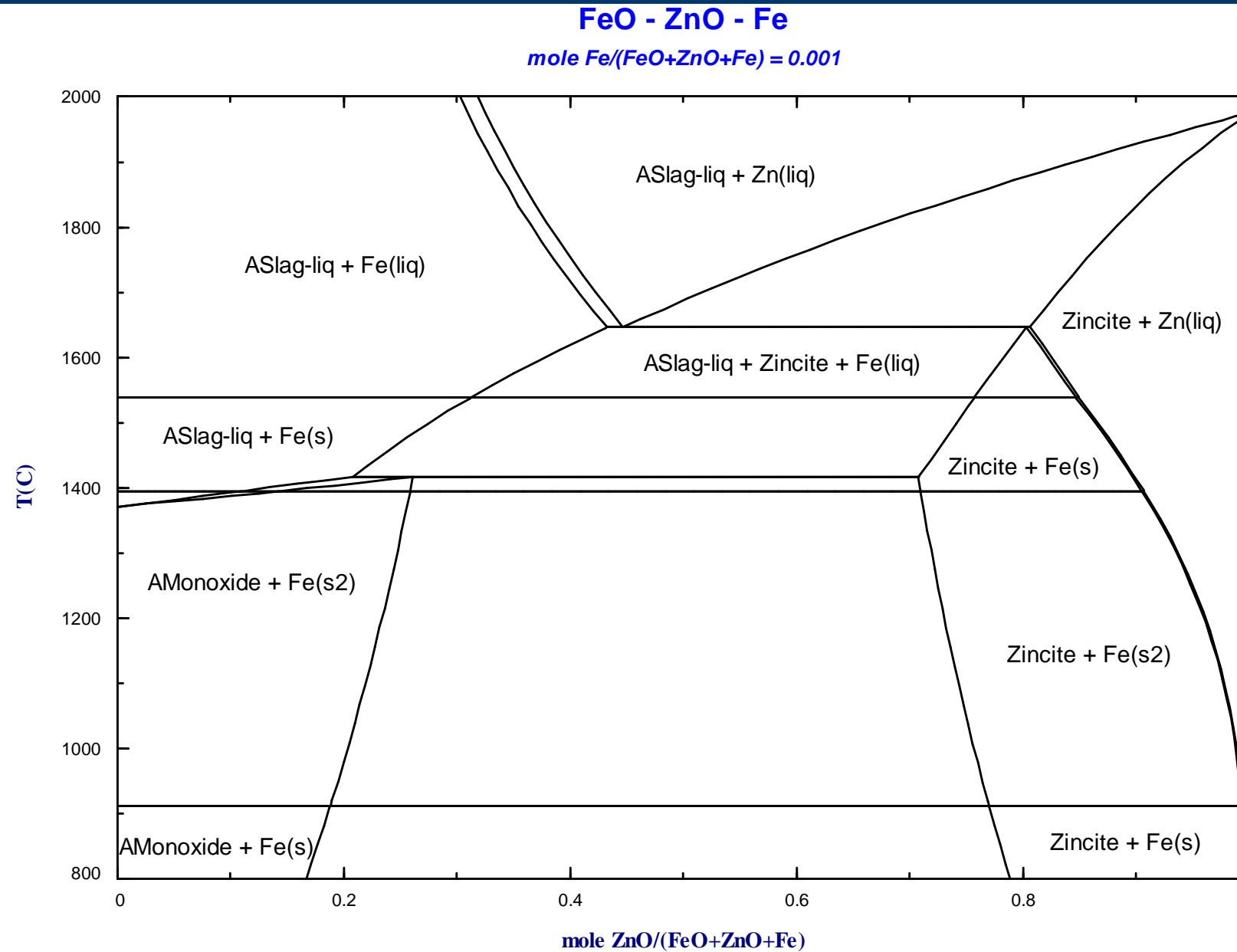
Oxide phases

Pure Fe and Zn (sol. and liq.) from Fact53

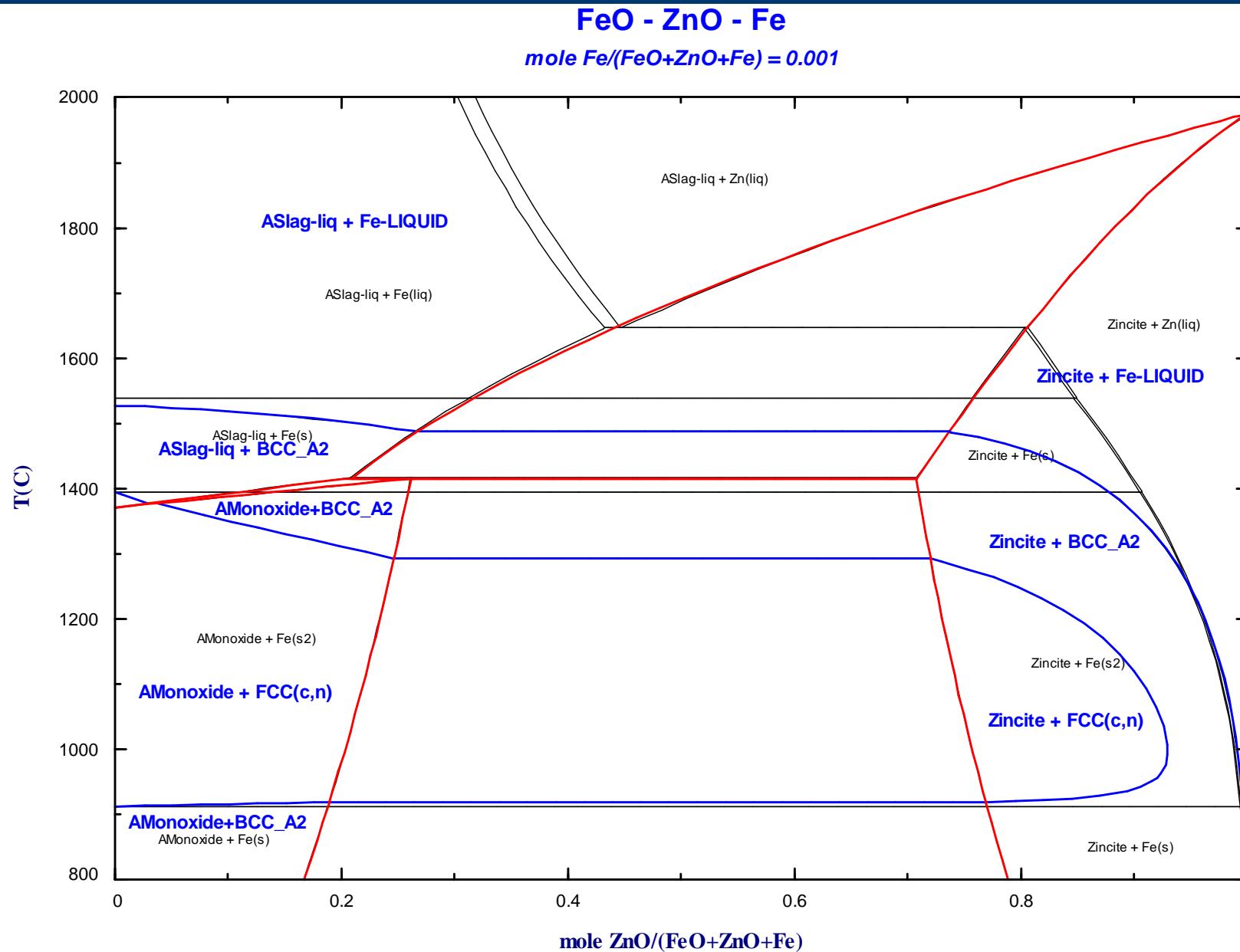
Oxides and Pyro

Show Selected | Select All | Select/Clear | Clear | OK

FeO-ZnO System in Equilibrium with Metals



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



FeO-ZnO System in Equilibrium with Metals and Gas

Data Search

Databases - 3/24 compound databases, 2/22 solution databases

Fact **FactSage™** **SGTE**

<input type="checkbox"/> ELEM	<input type="checkbox"/> FSropp	<input type="checkbox"/> BINS	<input type="checkbox"/> compounds only
<input type="checkbox"/> FACT	<input type="checkbox"/> FSlead	<input type="checkbox"/> SGPS	<input type="checkbox"/> solutions only
<input checked="" type="checkbox"/> Fact53	<input type="checkbox"/> FSlite	<input type="checkbox"/> SGTE	<input type="checkbox"/> no data
<input checked="" type="checkbox"/> FToxid	<input checked="" type="checkbox"/> FSstel	<input type="checkbox"/> SGnobl	
<input type="checkbox"/> FTsalt	<input type="checkbox"/> FSups	<input type="checkbox"/> SGsold	
<input type="checkbox"/> FTmisc	<input type="checkbox"/> FSnobl	<input type="checkbox"/> SGnucl	
<input type="checkbox"/> FThall			
<input type="checkbox"/> FTholg			
<input type="checkbox"/> FTpulp			
<input type="checkbox"/> FTlite			

Miscellaneous

<input type="checkbox"/> EXAM	<input type="checkbox"/> SGSL	<input type="checkbox"/> SGTE*
-------------------------------	-------------------------------	--------------------------------

Other

<input type="checkbox"/> TDnucl	<input type="checkbox"/> OLIC	<input type="checkbox"/> OLIL
<input type="checkbox"/> OLIP	<input type="checkbox"/> OLIG	

Clear All Select All Add/Remove Data RefreshDatabases

Information -

Oxide phases

Metal phases from FSstel

Gaseous species from Fact53

Options

Include:

gaseous ions (plasmas)
 aqueous species
 limited data compounds (25C)

Limits:

Organic species C_xH_y..., X(max) =
Minimum solution components: 1 2 cpts

Cancel Summary ... OK

FeO-ZnO System in Equilibrium with Metals and Gas

F Menu - Phase Diagram: FeO-ZnO at metal sat

File Units Parameters Variables Help

T(C) P(atm) Energy(J) Mass(mol) Vol(litre)

Components (3)

FeO + ZnO + Fe

Products

Compound species

- + gas ideal real 6
- aqueous 0
- pure liquids 0
- * + pure solids 7
- suppress duplicates
- * - custom selection species: 13

Target: none

Estimate T(K): 1000

Mass(mol): 0

Solution species

	Base-Phase	Full Name
*	+	FSstel-FEZ1
*	+	FSstel-FEZ2
*	+	FSstel-FEZ3
*	+	FSstel-HCP
I	FToxid-SLAGA	ASlag-liq
+	FToxid-SPINA	ASpinel
+	FToxid-MeO_A	AMonoxide
+	FToxid-ZNIT	Zincite

Legend: I - immiscible 1
+ - selected 12

Show all selected
species: 51
solutions: 14

Variables

T(C)	ZnO/(FeO+ZnO+Fe)	Fe/(FeO+ZnO+Fe)		
800 2000	0 1	0.001		

T(C) vs ZnO/(FeO+ZnO+Fe)

FactSage 6.2 beta g:\...\PhasFe-Zn-O_FeO-ZnO-Fe_FSstel_gas.DAT

Oxide phases, all Metal phases from FSstel

Gaseous species only from Fact53

F Selection - Equilib

Selected: 7/23 Duplicates selected SOLID Sorted by Code

	Code	Species	Data	Phase	T	V	Activity
+	23	Fe3O4(s2)	FACT53	magnetite		V	
+	24	Fe3O4(s3)	FACT53	high-pressure...		V	
+	25	Fe3O4(s4)	FACT53	high-pressure...		V	
+	26	Zn(s)	FACT53	solid			
+	27	ZnO(s)	FACT53	zincite			
+	28	ZnFe2O4(s)	FACT53	solid			
+	29	Fe(s)	FSstel	bcc_a2			
+	30	Fe(s2)	FSstel	fcc_a1			
+	31	Fe2O3(s)	FSstel	hematite	V		
+	32	Fe3O4(s)	FSstel	magnetite	V		
+	33	Fe3O4(s2)	FSstel	magnetite	V		
+	34	Zn(s)	FSstel	hcp_zn	o		
+	35	Fe2O3(s)	FToxid	hematite	V		
+	36	Fe2O3(s2)	FToxid	high-pressure...	V		
+	37	Fe2O3(s3)	FToxid	high-pressure...	V		
+	38	ZnO(s)	FToxid	zincite			

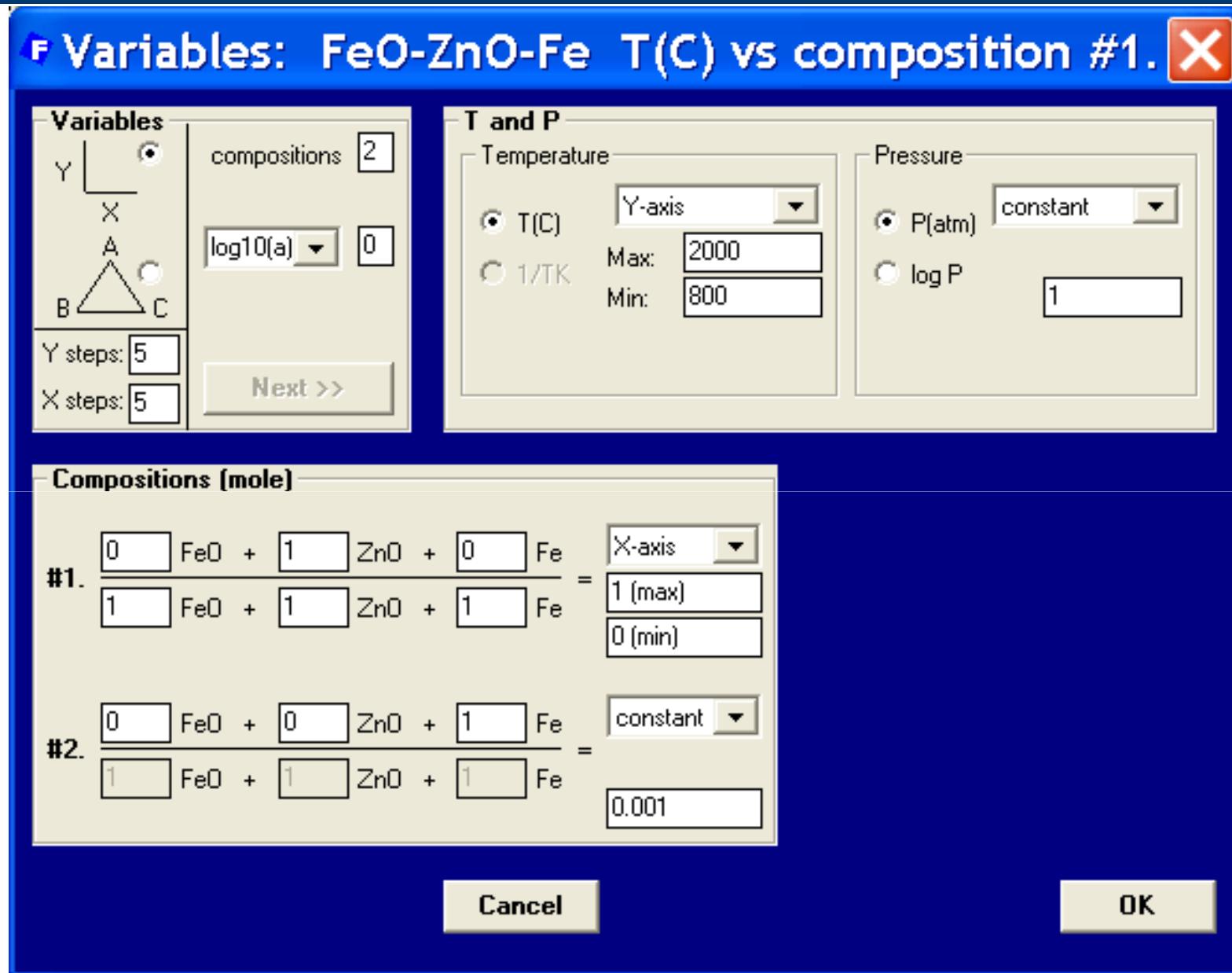
F Selection - Equilib

Selected: 6/6 GAS Sorted by Code

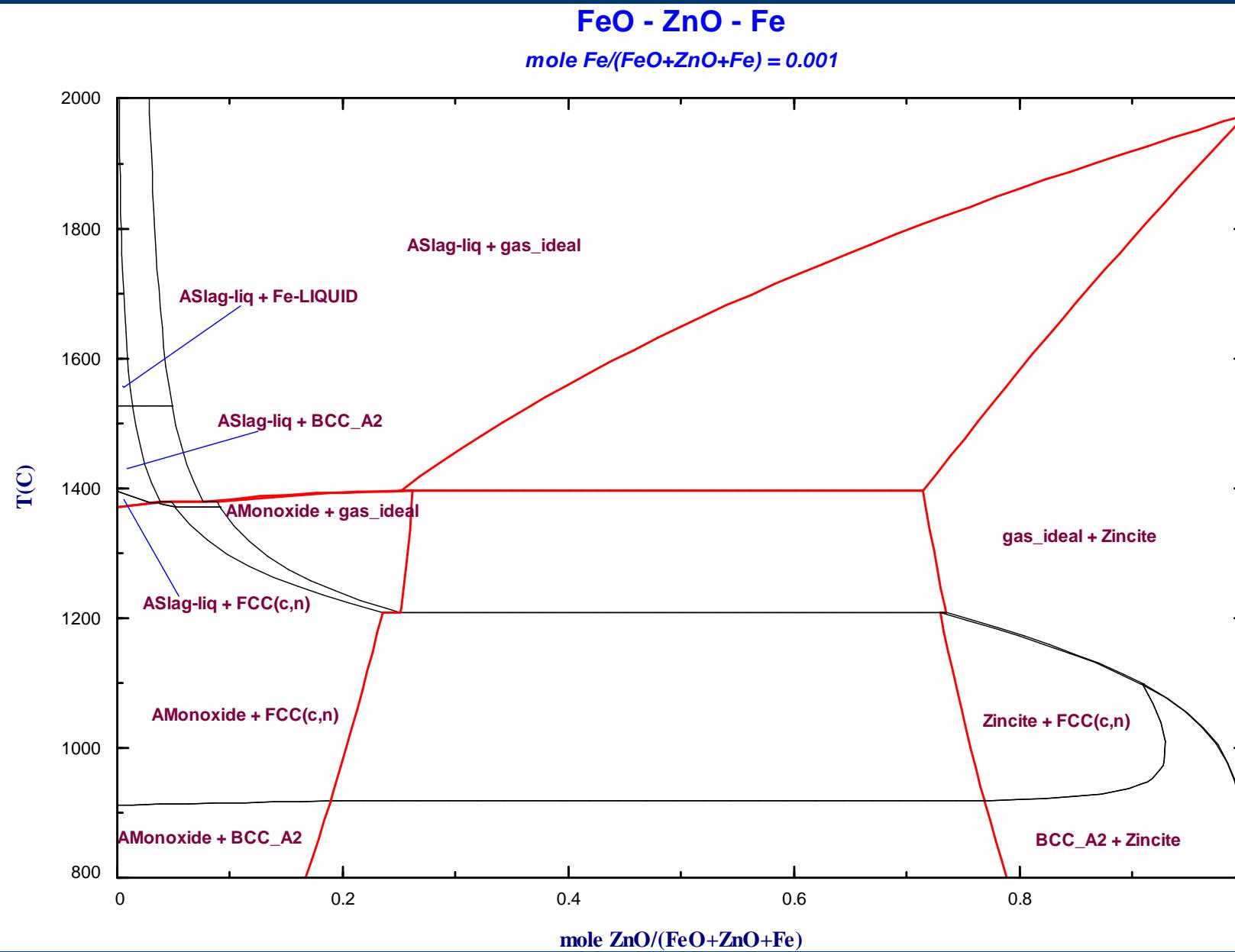
	Code	Species	Data	Phase	T	V	Activity
+	1	O(g)	FACT53	gas			
+	2	O2(g)	FACT53	gas			
+	3	O3(g)	FACT53	gas			
+	4	Fe(g)	FACT53	gas			
+	5	FeO(g)	FACT53	gas			
+	6	Zn(g)	FACT53	gas			

ow Selected Select All Select/Clear... Clear OK

FeO-ZnO System in Equilibrium with Metals and Gas

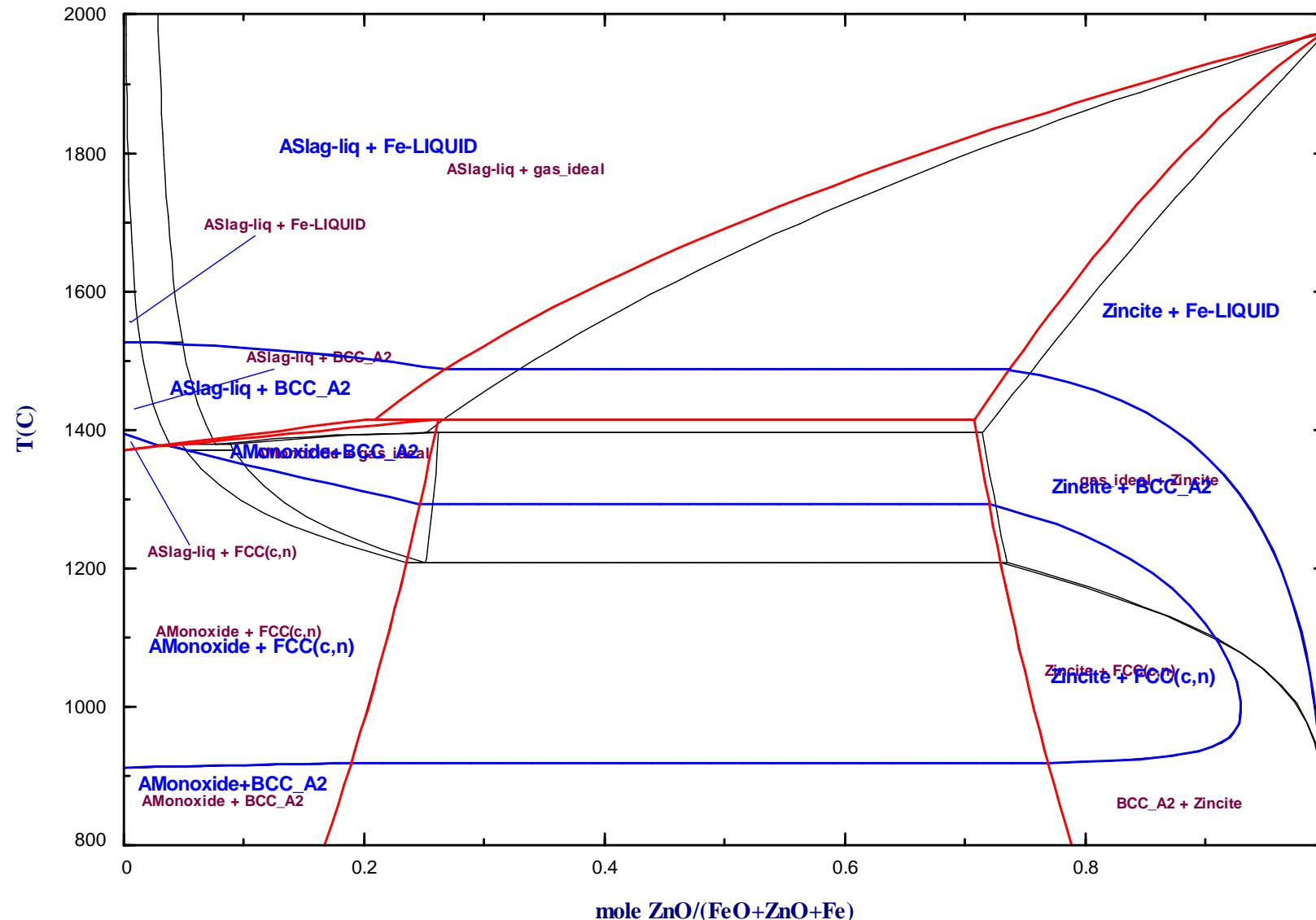


FeO-ZnO System in Equilibrium with Metals and Gas

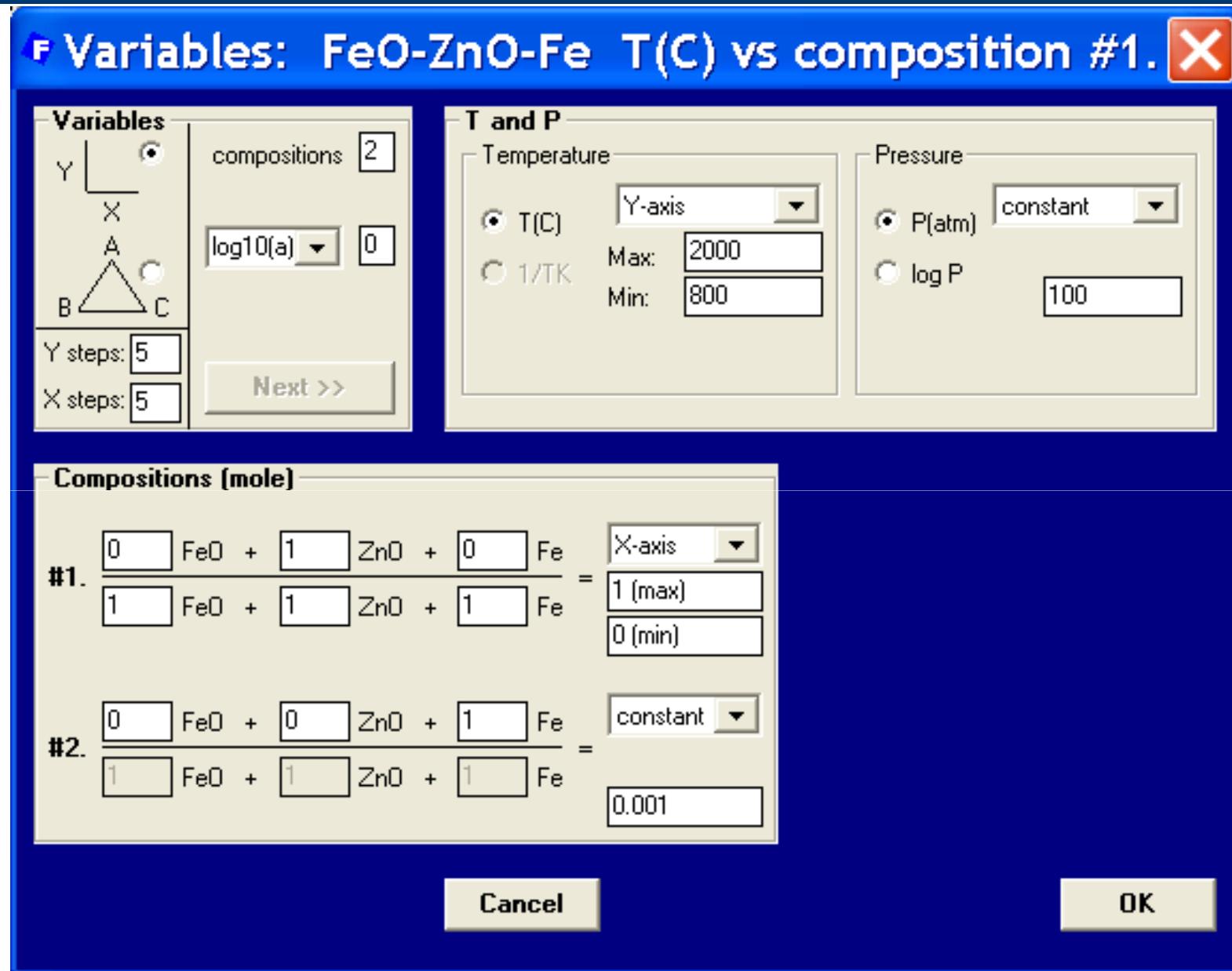


FeO-ZnO System in Equilibrium with Metals and Gas

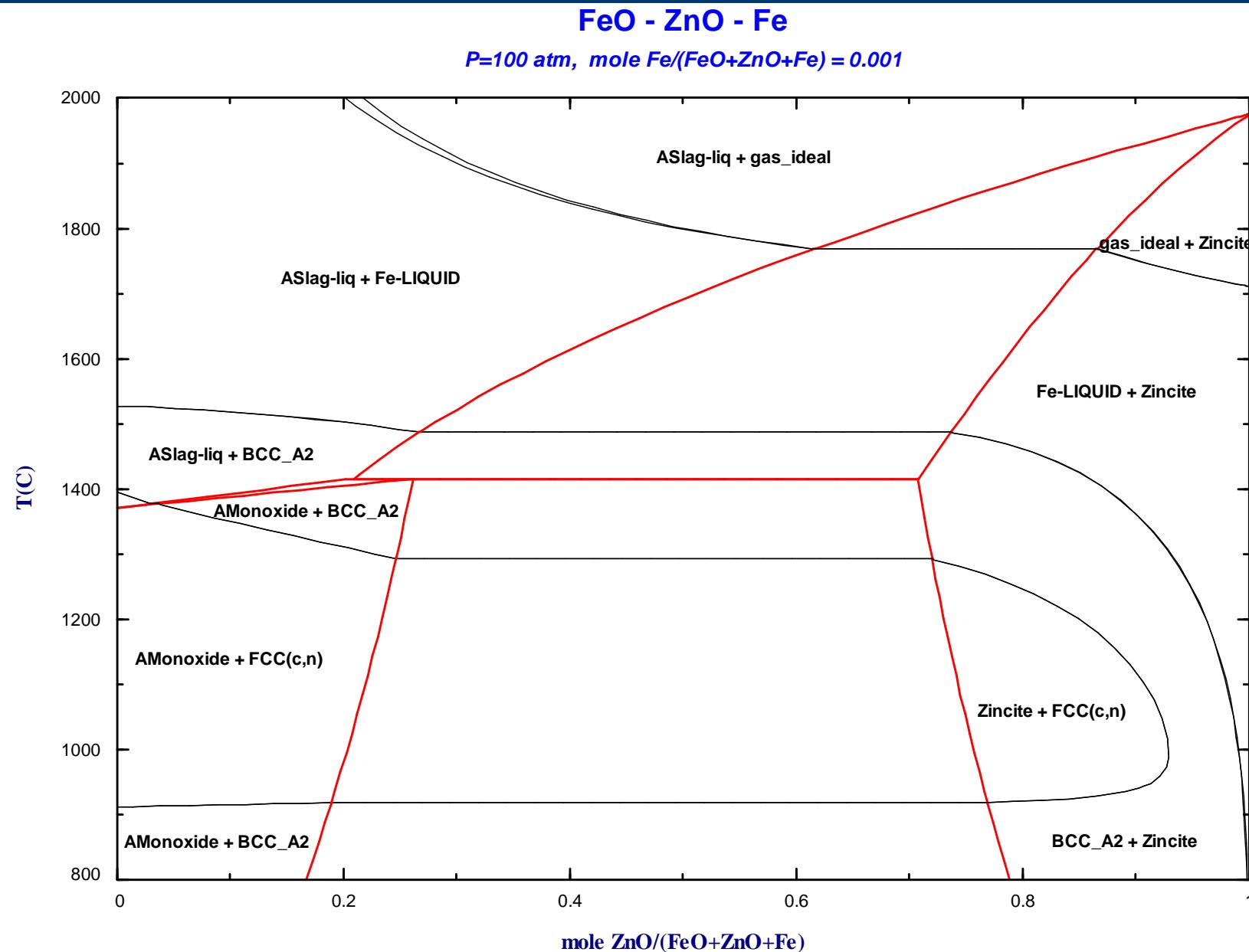
Red and blue curves are calculated without gas



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

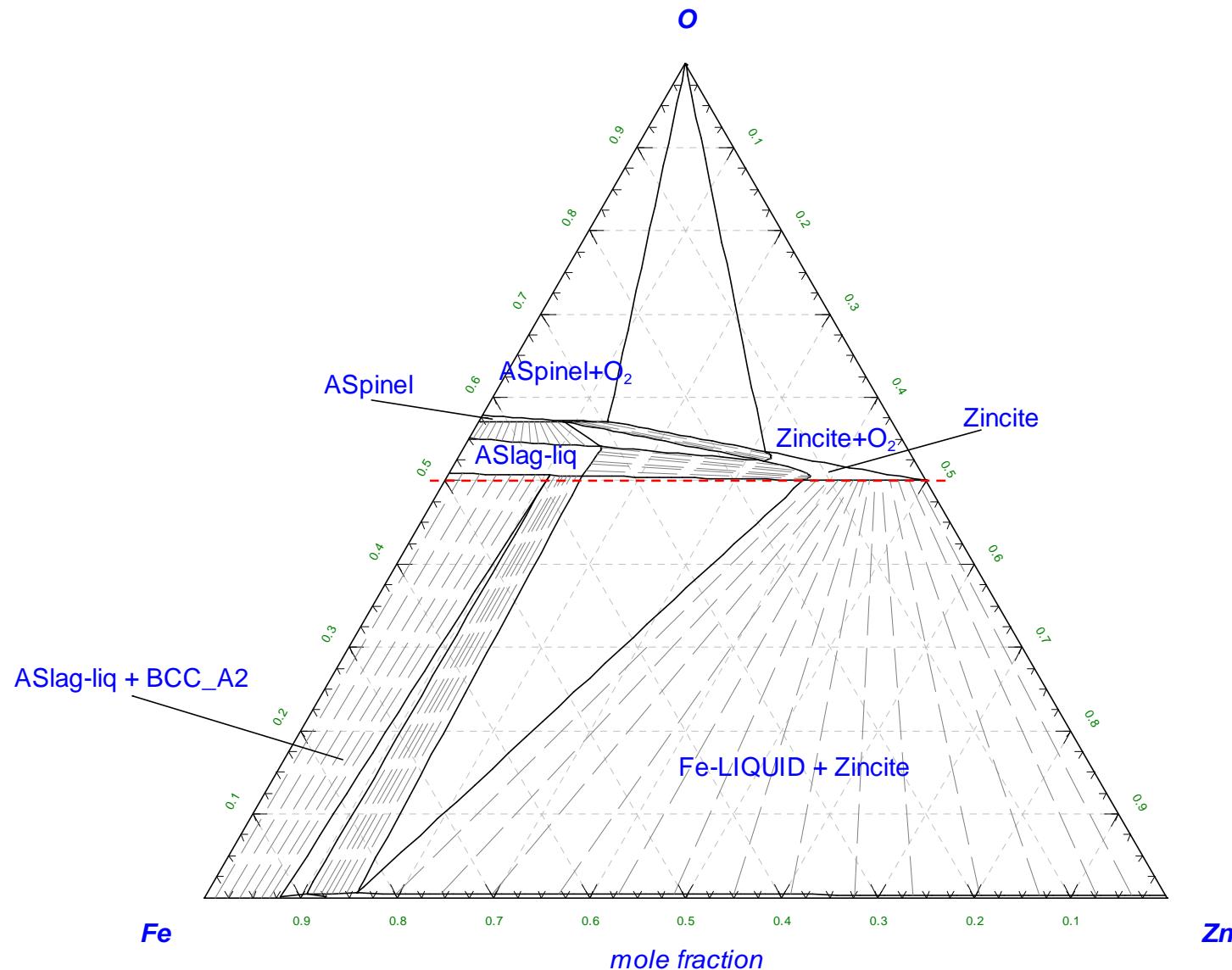


FeO-ZnO in Equilibrium with Metals at P=100 atm



Fe-Zn-O System

1500°C



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

File Edit Units Data Search Help

T(C) P(atm) Energy(J) Mass(mol) Vol(litre)

1 - 3

Components

FeO
CoO
Fe

Data Search

Databases - 3/24 compound databases, 2/22 solution databases

Fact **FactSage™** **SGTE**

<input type="checkbox"/> ELEM	<input type="checkbox"/> FSopp	<input type="checkbox"/> BINS	<input type="checkbox"/> compounds only
<input type="checkbox"/> FACT	<input type="checkbox"/> FLead	<input type="checkbox"/> SGPS	<input type="checkbox"/> solutions only
<input checked="" type="checkbox"/> Fact53	<input type="checkbox"/> FSite	<input type="checkbox"/> SGTE	<input type="checkbox"/> no data
<input checked="" type="checkbox"/> FToxic	<input checked="" type="checkbox"/> FSstel	<input type="checkbox"/> SGnobl	<input type="checkbox"/> EXAM
<input type="checkbox"/> FTsalt	<input type="checkbox"/> FSups	<input type="checkbox"/> SGsold	<input type="checkbox"/> SGSL
<input type="checkbox"/> FTmisc	<input type="checkbox"/> FSnobl	<input type="checkbox"/> SGnucl	<input type="checkbox"/> SGTE*
<input type="checkbox"/> FThall			<input type="checkbox"/> Clear All
<input type="checkbox"/> FTheig			<input type="checkbox"/> Select All
<input type="checkbox"/> FTPulp		<input type="checkbox"/> TDnucl	<input type="checkbox"/> Add/Remove Data
<input type="checkbox"/> FTlite	<input type="checkbox"/> OLIP	<input type="checkbox"/> OLIC	<input type="checkbox"/> RefreshDatabases
	<input type="checkbox"/> OLIG	<input type="checkbox"/> OLIL	

Miscellaneous

EXAM SGSL SGTE*

Clear All
 Select All
 Add/Remove Data
 RefreshDatabases

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).

If database is stored on your PC but not listed here then you must 'add the database to the list' - click on 'Add/Remove ..'.

Options

Default

Include
 gaseous ions
(in plasma)
 aqueous species
 limited data compounds (25C)

Limits
Organic species CxHy... X(max) =
Minimum solution components: 1 2 cpts

Cancel Summary ... OK

FactSage 6.2 beta Compound: 3/24 databases Solution: 2/22 databases

Oxide phases, Gaseous species

Metal phases from FSstel

FeO-CoO System in Equilibrium with Metals

F Menu - Phase Diagram: FeO-CoO-Fe at metal saturation using ... - X

File Units Parameters Variables Help

T(C) P(atm) Energy(J) Mass(mol) Vol(litre)

Components (3)

FeO + CoO + Fe

Products

Compound species

<input type="checkbox"/> gas	<input checked="" type="radio"/> ideal	<input type="radio"/> real	6
<input type="checkbox"/> aqueous	0		
<input type="checkbox"/> pure liquids	0		
<input checked="" type="checkbox"/> pure solids	11		
<input type="checkbox"/> suppress duplicates		<input type="button" value="apply"/>	
*- custom selection			
species: 17			

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)
I	FToxid-SLAGA	ASlag-liq	
	+	FToxid-SPINA	ASpinel
I	FToxid-MeO_A	AMonoxide	

Custom Solutions

0 fixed activities
0 ideal solutions
0 activity coefficients

Details ...

Pseudonyms

apply List ...

include molar volumes

Total Species (max 1500) 58
Total Solutions (max 40) 9

Legend

I - immiscible 2
+ - selected 5

Show all selected

species: 41
solutions: 9

Variables

T(C)	CoO/(FeO+CoO)	Fe/(FeO+CoO)		
100 1300	0.1	0.001		

T(C) vs CoO/(FeO+CoO)

Phase Diagram

Y Calculate >>
X

FactSage 6.2 beta C:\...\PhasCo-Fe-O_FeO-CoO-Fe_FSstel.DAT

FeO-CoO System in Equilibrium with Metals

F Variables: FeO-CoO-Fe T(C) vs composition #1.



Variables

compositions 2
 $\log_{10}(a)$ 0
Y steps: 5
X steps: 5

T and P

Temperature: Y-axis, Max: 1300, Min: 100
Pressure: constant, P(atm), log P: 1

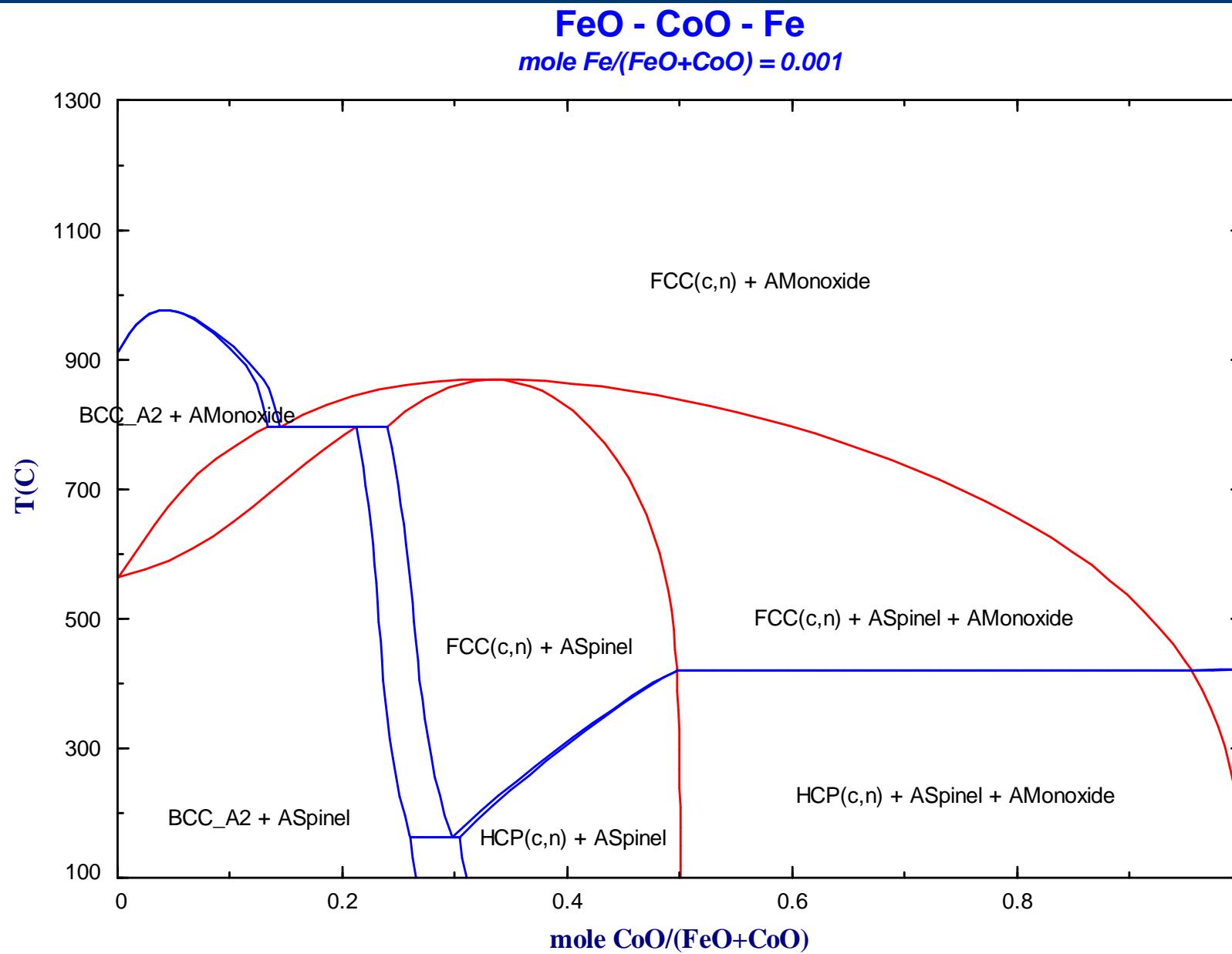
Compositions (mole)

#1. $0 \text{ FeO} + 1 \text{ CoO} + 0 \text{ Fe} = \text{X-axis}$
1 (max)
0 (min)

#2. $0 \text{ FeO} + 0 \text{ CoO} + 1 \text{ Fe} = \text{constant}$
0.001

Cancel OK

FeO-CoO System in Equilibrium with Metals



FeO-CoO System in Equilibrium with Pure Fe and Co

F Data Search

Databases - 2/24 compound databases, 1/22 solution databases

Fact **FactSage™** **SGTE**

<input type="checkbox"/> ELEM	<input type="checkbox"/> FScopp	<input type="checkbox"/> BINS	<input type="checkbox"/> compounds only
<input type="checkbox"/> FACT	<input type="checkbox"/> FSLead	<input type="checkbox"/> SGPS	<input type="checkbox"/> solutions only
<input checked="" type="checkbox"/> Fact53	<input type="checkbox"/> FSlite	<input type="checkbox"/> SGTE	<input type="checkbox"/> no data
<input checked="" type="checkbox"/> FToxid	<input type="checkbox"/> FSstel	<input type="checkbox"/> SGnobl	
<input type="checkbox"/> FTsalt	<input type="checkbox"/> FSups	<input type="checkbox"/> SGsold	
<input type="checkbox"/> FTmisc	<input type="checkbox"/> FSnobl	<input type="checkbox"/> SGnucl	
<input type="checkbox"/> FThall			
<input type="checkbox"/> FThelg			
<input type="checkbox"/> FTpulp	<input type="checkbox"/> OLIP	<input type="checkbox"/> TDnucl	
<input type="checkbox"/> FTlite	<input type="checkbox"/> OLIG	<input type="checkbox"/> OLIC	
		<input type="checkbox"/> OLIL	

Miscellaneous

EXAM SGSL SGTE*

Information - Including aqueous species is only meaningful in aqueous (hydrometallurgical) calculations at or near room temperature. If your calculations are above 300 C there is no point in including the aqueous species. This option has no effect upon gaseous ions (plasmas).

Oxide phases, Gaseous species

Metal phases from Fact53

Options

Include:

gaseous ions
 (plasma)
 aqueous species
 limited data compounds (25C)

Limits

Organic species CxHy... X(max) =

Minimum solution components: 1 2 cpts

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)

Components (3)

FeO + CoO + Fe

Products

Compound species

- + gas ideal real 6
- aqueous 0
- pure liquids 0
- * + pure solids 6
- suppress duplicates

* - custom selection species: 12

Target - none -

Estimate T(K): 1000

Mass(mol): 0

Legend I- immiscible 1 + selected 2

Show all selected

species: 29 solutions: 4

Solution species

*	+	Base-Phase	Full Name
	I	FToxic-SLAGA	ASlag-liq
	+	FToxic-SPINA	ASpinel
	+	FToxic-MeO_A	AMonoxide

F Selection - Equilib

File Edit Show Sort

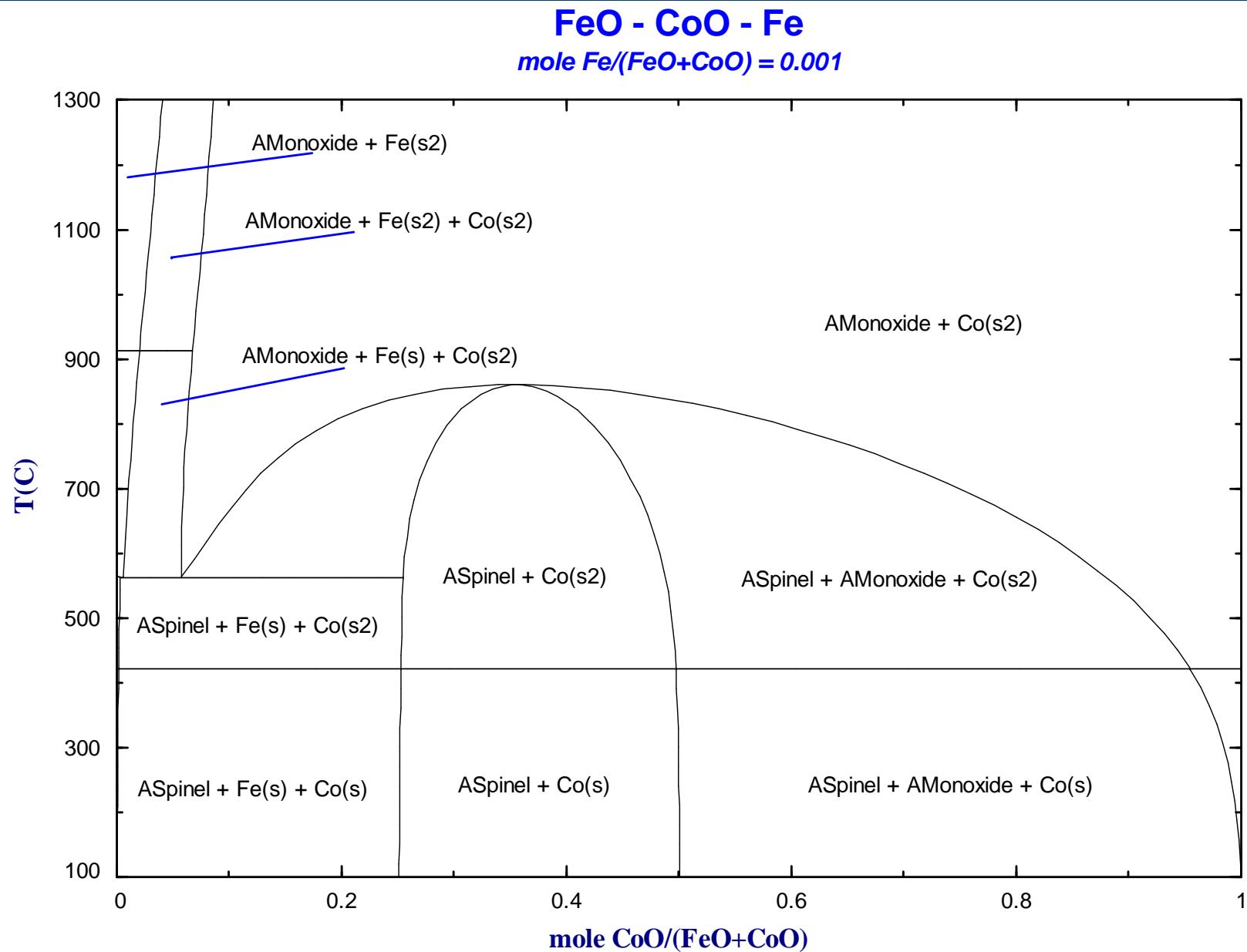
Selected: 8/19 Duplicates selected. SOLID Sorted by Code

+	Code	Species	Data	Phase	T	V	Activity
+	13	Fe(s)	FACT53	bcc			
+	14	Fe(s2)	FACT53	fcc			
	15	FeO(s)	FACT53	wustite		V	
	16	Fe2O3(s)	FACT53	hematite		V	
	17	Fe2O3(s2)	FACT53	high-pressure		V	
	18	Fe2O3(s3)	FACT53	high-pressure		V	
	19	Fe3O4(s)	FACT53	magnetite		V	
	20	Fe3O4(s2)	FACT53	magnetite		V	
	21	Fe3O4(s3)	FACT53	high-pressure		V	
	22	Fe3O4(s4)	FACT53	high-pressure		V	
+	23	Co(s)	FACT53	solid			
+	24	Co(s2)	FACT53	solid			
	25	CoO(s)	FACT53	solid			
	26	Co3O4(s)	FACT53	solid			
	27	(CoO)(Fe2O3)(s)	FACT53	solid		o	
+	28	Fe2O3(s)	FToxic	hematite		V	
+	29	Fe2O3(s2)	FToxic	high-pressure		V	
+	30	Fe2O3(s3)	FToxic	high-pressure		V	
+	31	CoO(s)	FToxic	solid			

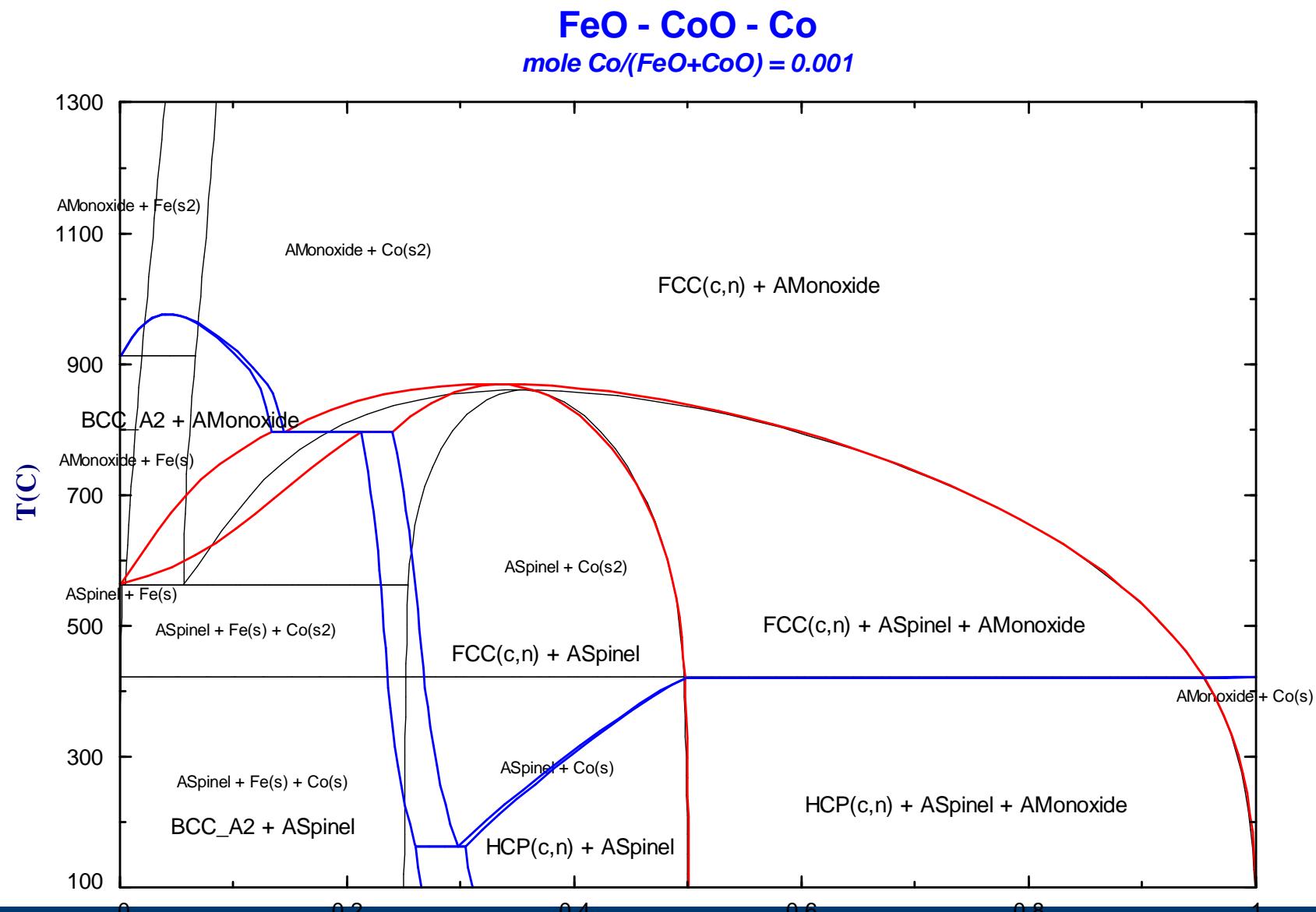
Oxide phases

Fe and Co from Fact53

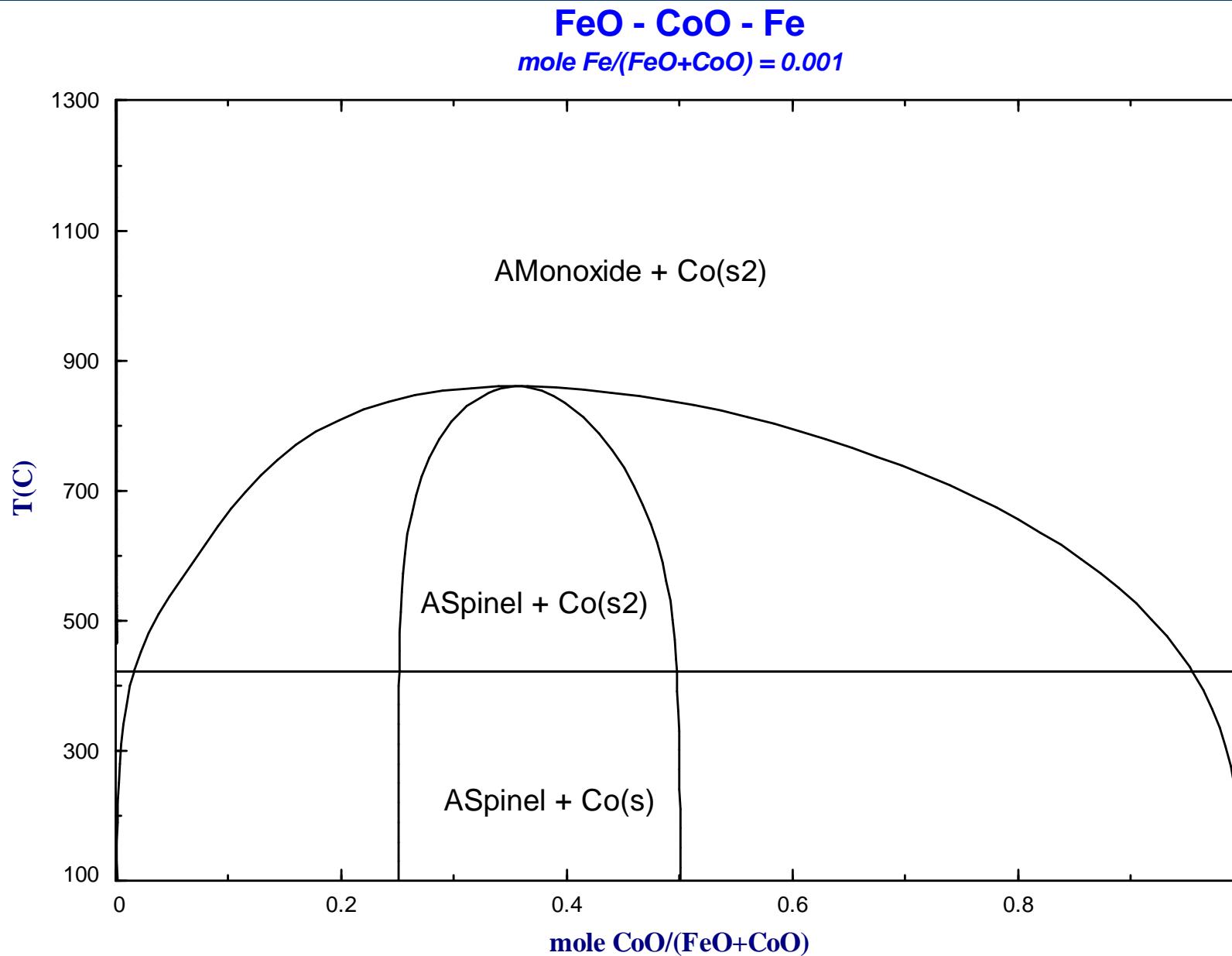
FeO-CoO System in Equilibrium with Pure Fe and Co



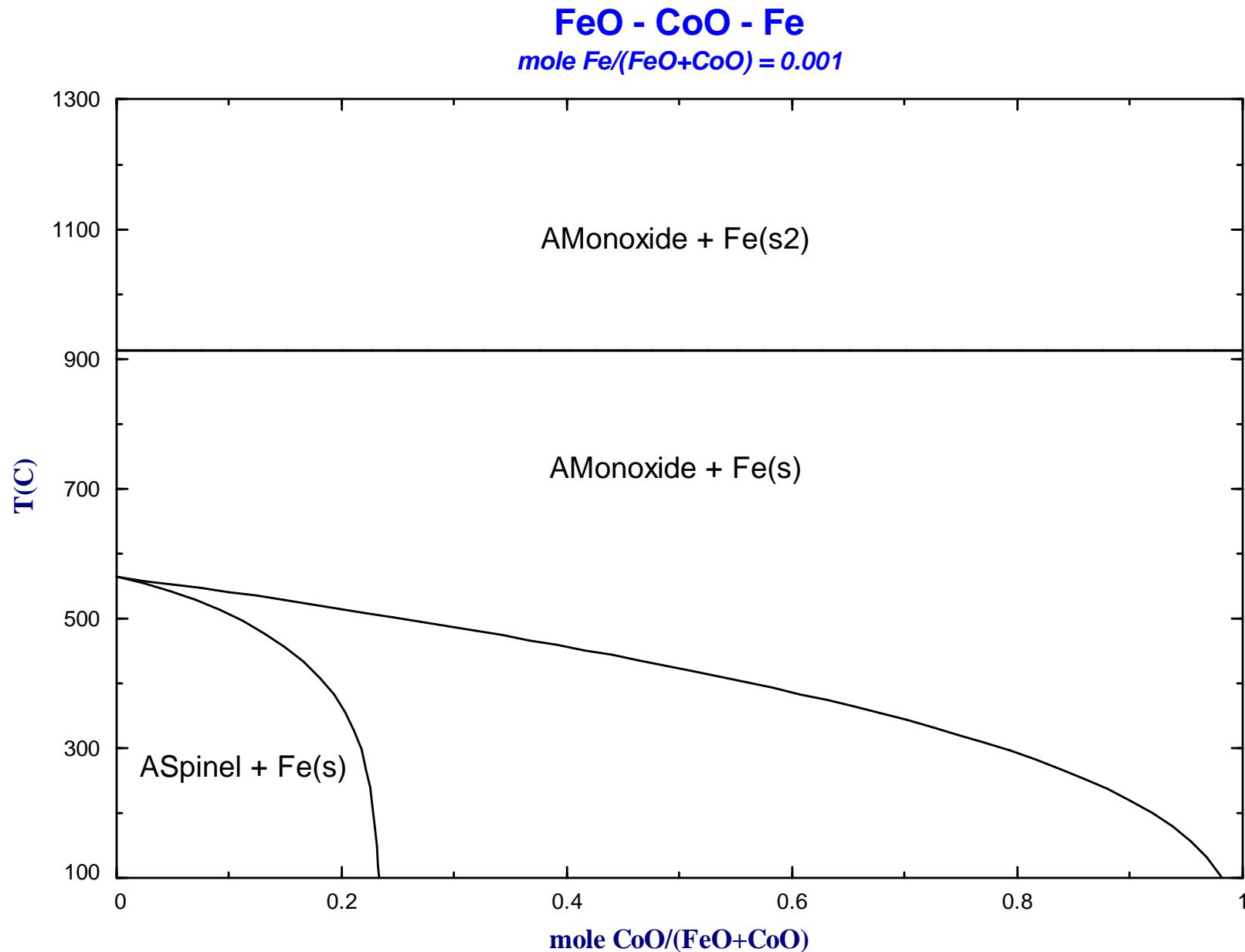
FeO-CoO in Equilibrium with Fe and Co vs FSstel



FeO-CoO System in Equilibrium with Pure Co



FeO-CoO System in Equilibrium with Pure Fe



Fe-Co-O System in Equilibrium with Metals

F Menu - Phase Diagram: Using FSstel for metallic phases

File Units Parameters Variables Help

T(C) P(atm) Energy(J) Mass(mol) Vol(litre)

Components (3) Fe + Co + O

Products

Compound species

- * gas ideal real 1
- aqueous 0
- pure liquids 0
- * pure solids 4
- suppress duplicates

* - 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)
I		FToxid-SLAGA	ASlag-liq
	+	FToxid-SPINA	ASpinel
	+	FToxid-MeO_A	AMonoxide

Custom Solutions

- 0 fixed activities
- 0 ideal solutions
- 0 activity coefficients

Pseudonyms

apply

include molar volumes

Total Species (max 1500) 43
Total Solutions (max 40) 8

Legend

I - immiscible 1
++ - selected 6

Show all selected
species: 38
solutions: 8

Variables

T(C)	O/(Fe+Co+O)	Co/(Fe+Co+O)		
700	0 1	0 1		

A = O, B = Fe, C = Co

Phase Diagram

Calculate >

FactSage 6.2 beta C:\CAD\...\All Diagrams\PhasCo-Fe-O_700C_FSstel.DAT

Fe-Co-O System in Equilibrium with Metals

F Variables: Fe-Co-O composition #1. vs composition #1. X

Variables

Y (radio button selected) compositions (2)
 $\log_{10}(a)$: 0
Y steps: 5 X steps: 5
Next >>

T and P

Temperature: constant T(C) 700
Pressure: constant P(atm) 1
 $\log P$

Compositions (mole)

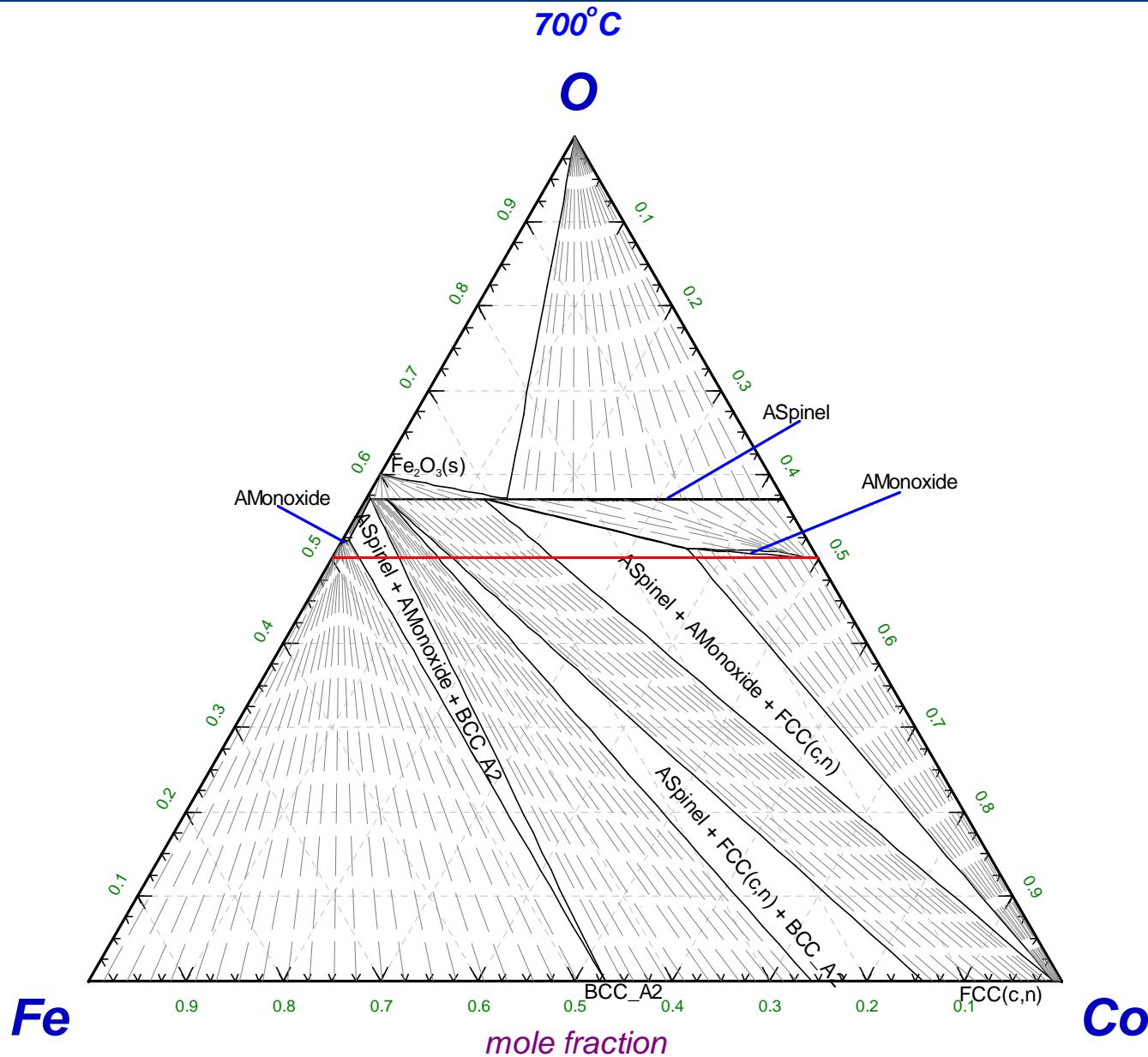
#1. $\frac{0 \text{ Fe} + 0 \text{ Co} + 1 \text{ O}}{1 \text{ Fe} + 1 \text{ Co} + 1 \text{ O}} =$ A-Corner
1 (max)
0 (min)

#2. $\frac{0 \text{ Fe} + 1 \text{ Co} + 0 \text{ O}}{1 \text{ Fe} + 1 \text{ Co} + 1 \text{ O}} =$ C-Corner
1 (max)
0 (min)

#3. $\frac{1 \text{ Fe} + 0 \text{ Co} + 0 \text{ O}}{1 \text{ Fe} + 1 \text{ Co} + 1 \text{ O}} =$ B-Corner
1 (max)
0 (min)

Cancel **OK**

Fe-Co-O System in Equilibrium with Metals



Fe-Co-O System in Equilibrium with Pure Metals

F Menu - Phase Diagram: last system

File Units Parameters Variables Help

T(C) P(atm) Energy(J) Mass(mol) Vol(litre)

Components (3) Fe + Co + O

Products

Compound species	+ gas	<input checked="" type="radio"/> ideal	<input type="radio"/> real	6
aqueous	0			
* pure liquids	2			
* pure solids	8			
<input type="checkbox"/> suppress duplicates	<input type="button" value="apply"/>			
* - custom selection				
species:	16			

Solution species

*	+	Base-Phase	Full Name
	I	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 2

Show all selected
species: 29
solutions: 4

Variables

T(C)	O/(Fe+Co+O)	Co/(Fe+Co+O)		
700	0.1	0.1		

A = O, B = Fe, C = Co

FactSage 6.2 beta

F Selection - Equilib

Selected: 8/19 Duplicates selected SOLID Sorted by Code

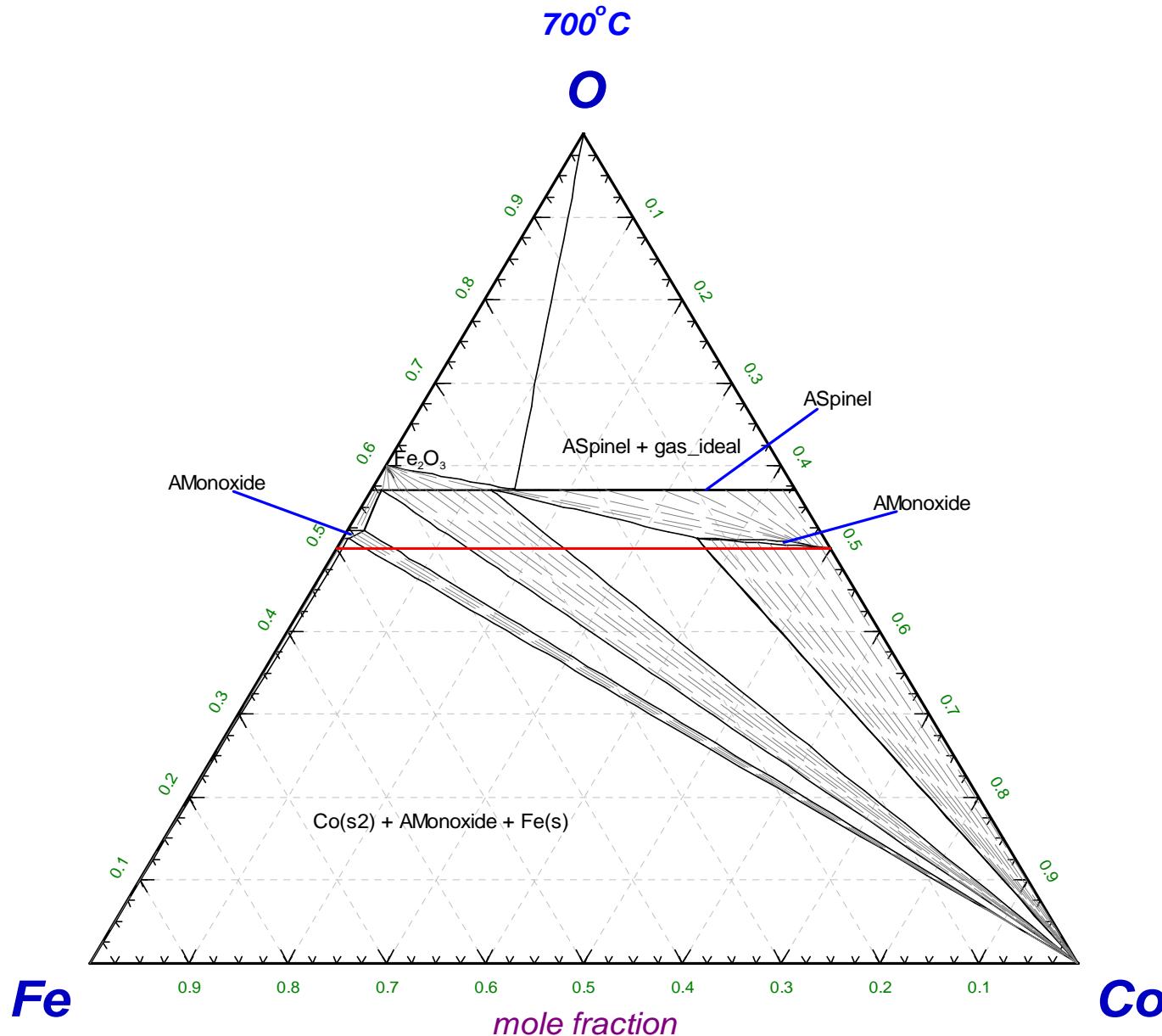
+	Code	Species	Data	Phase	T	V	Activity
+	13	Fe(s)	FACT53	bcc			
+	14	Fe(s2)	FACT53	fcc			
	15	FeO(s)	FACT53	wustite		V	
	16	Fe2O3(s)	FACT53	hematite		V	
	17	Fe2O3(s2)	FACT53	high-pressure		V	
	18	Fe2O3(s3)	FACT53	high-pressure		V	
	19	Fe3O4(s)	FACT53	magnetite		V	
	20	Fe3O4(s2)	FACT53	magnetite		V	
	21	Fe3O4(s3)	FACT53	high-pressure		V	
	22	Fe3O4(s4)	FACT53	high-pressure		V	
+	23	Co(s)	FACT53	solid			
+	24	Co(s2)	FACT53	solid			
	25	CoO(s)	FACT53	solid			
	26	Co3O4(s)	FACT53	solid			
	27	(CoO)(Fe2O3)(s)	FACT53	solid		o	
+	28	Fe2O3(s)	FToxid	hematite		V	
+	29	Fe2O3(s2)	FToxid	high-pressure		V	
+	30	Fe2O3(s3)	FToxid	high-pressure		V	
+	31	CoO(s)	FToxid	solid			

Show Selected Select All Select/Clear... Clear OK

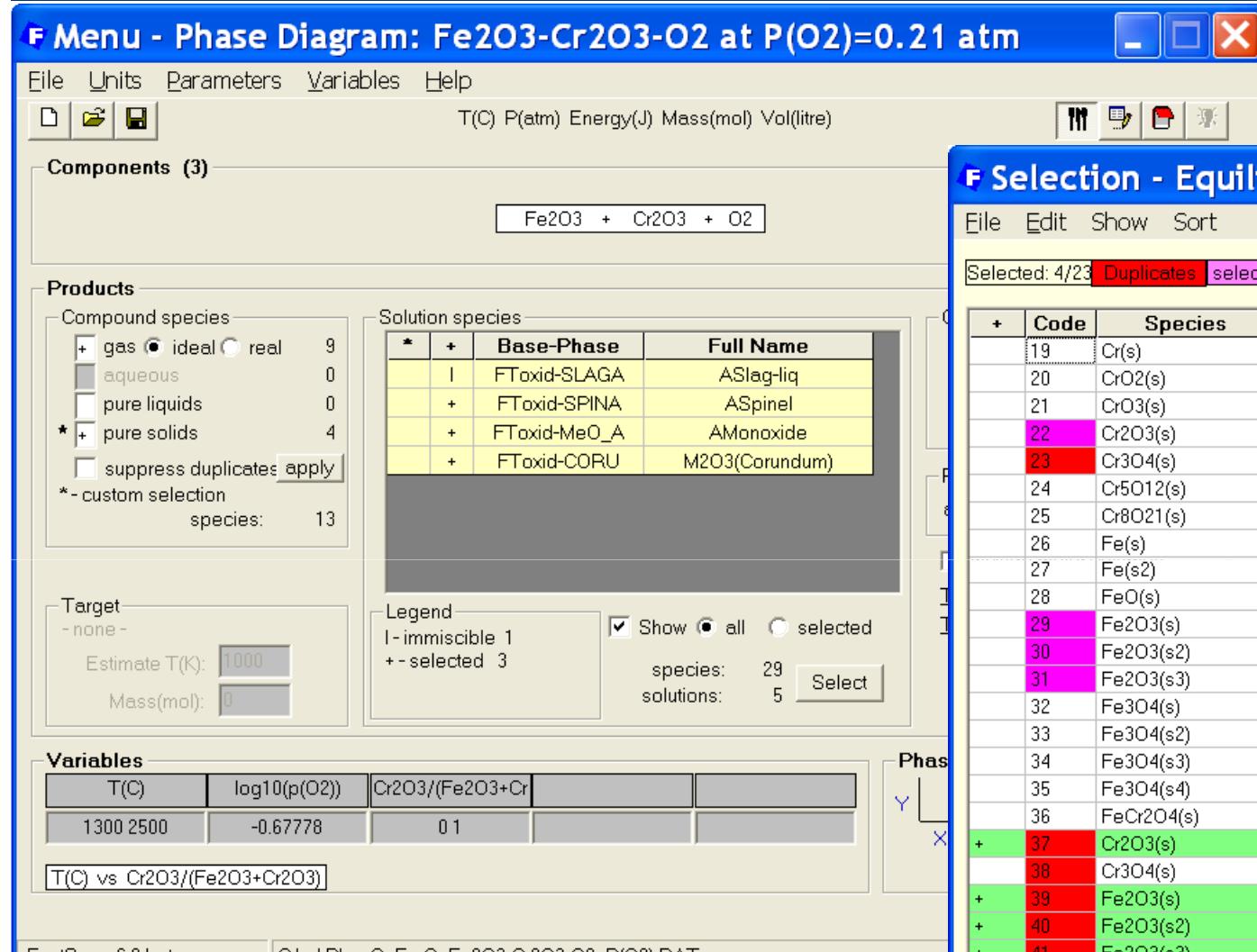
Oxide phases

Fe and Co from Fact53

Fe-Co-O System in Equilibrium with Pure Metals



Fe₂O₃-Cr₂O₃ System in Equilibrium with Air



Gas phase must be selected even though it does not form

F Selection - Equilib

File Edit Show Sort

Selected: 4/23 Duplicates selected. SOLID Sorted by Code

+	Code	Species	Data	Phase	T	V	Activity
	19	Cr(s)	FACT53	solid			
	20	CrO ₂ (s)	FACT53	solid		o	
	21	CrO ₃ (s)	FACT53	solid			
	22	Cr ₂ O ₃ (s)	FACT53	solid			
	23	Cr ₃ O ₄ (s)	FACT53	solid	o		
	24	Cr ₅ O ₁₂ (s)	FACT53	solid		o	
	25	Cr ₈ O ₂₁ (s)	FACT53	solid		o	
	26	Fe(s)	FACT53	bcc			
	27	Fe(s2)	FACT53	fcc			
	28	FeO(s)	FACT53	wustite	v		
	29	Fe ₂ O ₃ (s)	FACT53	hematite	v		
	30	Fe ₂ O ₃ (s2)	FACT53	high-pressure...	v		
	31	Fe ₂ O ₃ (s3)	FACT53	high-pressure...	v		
	32	Fe ₃ O ₄ (s)	FACT53	magnetite	v		
	33	Fe ₃ O ₄ (s2)	FACT53	magnetite	v		
	34	Fe ₃ O ₄ (s3)	FACT53	high-pressure...	v		
	35	Fe ₃ O ₄ (s4)	FACT53	high-pressure...	v		
	36	FeCr ₂ O ₄ (s)	FACT53	solid			
+	37	Cr ₂ O ₃ (s)	FToxid	solid			
	38	Cr ₃ O ₄ (s)	FToxid	solid	o		
+	39	Fe ₂ O ₃ (s)	FToxid	hematite	v		
+	40	Fe ₂ O ₃ (s2)	FToxid	high-pressure...	v		
+	41	Fe ₂ O ₃ (s3)	FToxid	high-pressure...	v		

Fe_2O_3 - Cr_2O_3 System in Equilibrium with Air

F Variables: Fe_2O_3 - Cr_2O_3 - O_2 T(C) vs composition #1.

Variables

Y (radio button selected)
X
A
B C
Y steps: 5
X steps: 5

compositions 1
 $\log_{10}(a)$ 1
Next >>

T and P

Temperature
T(C) (radio button selected)
1/T(K)
Y-axis
Max: 2500
Min: 1300

Pressure
P(atm) (radio button selected)
constant 1
 $\log P$

Chemical Potentials

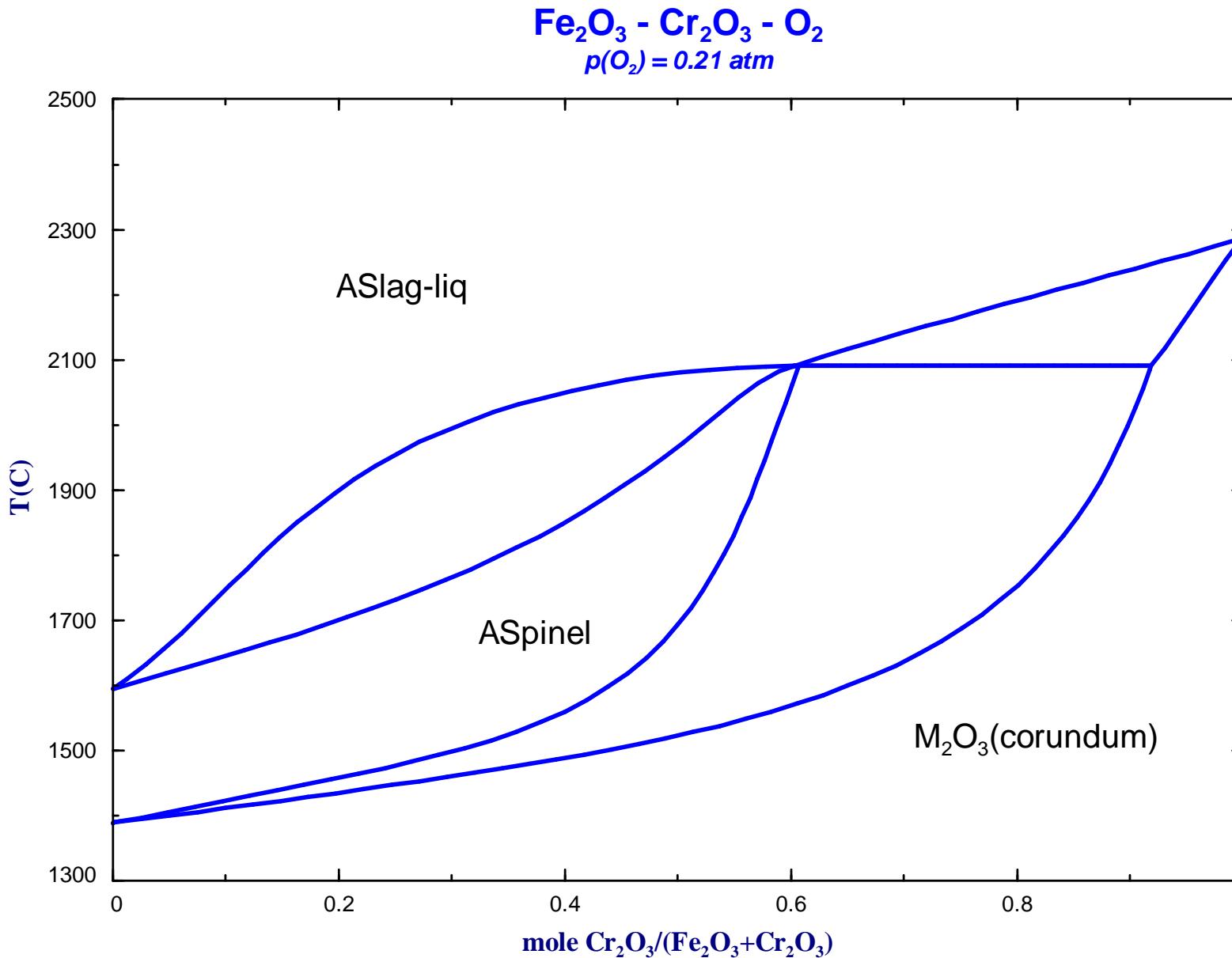
#1. $\log_{10}(p)$ = constant
O2
gas-FACT53 -0.67778

Compositions (mole)

#1. $\frac{0}{1} \text{ Fe}_2\text{O}_3 + \frac{1}{1} \text{ Cr}_2\text{O}_3 = \frac{1}{0} \text{ (max)} \text{ Fe}_2\text{O}_3 + \frac{1}{0} \text{ (min)} \text{ Cr}_2\text{O}_3$

Cancel OK

Fe_2O_3 - Cr_2O_3 System in Equilibrium with Air



MgO-Cr₂O₃ System at $P(O_2)=10^{-5.5}$ atm

F Menu - Phase Diagram: MgO-Cr₂O₃-O₂ at lgP(O₂)=-5.5

File Units Parameters Variables Help

T(C) P(atm) Energy(J) Mass(mol) Vol(litre)

Components (3)

MgO + Cr₂O₃ + O₂

Products

Compound species

- + gas ideal real 10
- aqueous 0
- pure liquids 0
- * pure solids 2
- suppress duplicates

* - custom selection

species: 12

Solution species

*	+	Base-Phase	Full Name
	I	FToxid-SLAGA	ASlag-liq
	+	FToxid-SPINA	ASpinel
	+	FToxid-MeO_A	AMonoxide

Target
- none -

Estimate T(K): 1000

Mass(mol): 0

Variables

T(C)	log10(p(O ₂))	Cr ₂ O ₃ /(MgO+Cr ₂ O ₃)		
1000 3000	-5.5	0.1		

T(C) vs Cr₂O₃/(MgO+Cr₂O₃)

FactSage 6.2 beta C:\...\PhasCr-Mg-O_MgO-Cr₂O₃-O₂_P(O₂).DAT

F Selection - Equilib

Selected: 2/13 Duplicates selected SOLID Sorted by Code

+	Code	Species	Data	Phase	T	V	Activity
20	Mg(s)	FACT53	solid				
21	MgO(s)	FACT53	periclase		V		
22	Cr(s)	FACT53	solid				
23	CrO ₂ (s)	FACT53	solid		o		
24	CrO ₃ (s)	FACT53	solid				
25	Cr ₂ O ₃ (s)	FACT53	solid				
26	Cr ₃ O ₄ (s)	FACT53	solid		o		
27	Cr ₅ O ₁₂ (s)	FACT53	solid		o		
28	Cr ₈ O ₂₁ (s)	FACT53	solid		o		
29	(MgO)(Cr ₂ O ₃)(s)	FACT53	chromite				
30	MgO(s)	FToxid	periclase		V		
31	Cr ₂ O ₃ (s)	FToxid	solid				

F Selection - Equilib

Selected: 10/10 GAS Sorted by Code

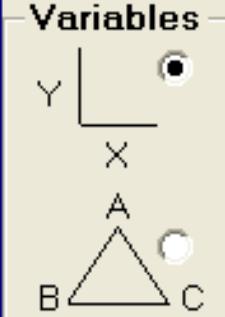
+	Code	Species	Data	Phase	T	V	Activity
1	O(g)	FACT53	gas				
2	O ₂ (g)	FACT53	gas				
3	O ₃ (g)	FACT53	gas				
4	Mg(g)	FACT53	gas				
5	Mg ₂ (g)	FACT53	gas				
6	MgO(g)	FACT53	gas				
7	Cr(g)	FACT53	gas				
8	CrO(g)	FACT53	gas				
9	CrO ₂ (g)	FACT53	gas				
10	CrO ₃ (g)	FACT53	gas				

Low Selected Select All Select/Clear... Clear OK

MgO-Cr₂O₃ System at $P(O_2)=10^{-5.5}$ atm

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

Variables

Y compositions 1
X
A
B 
C
Y steps: 5
X steps: 5
Next >>

T and P

Temperature
Y-axis T(C)
Max: 3000
Min: 1000
1/TK

Pressure
P(atm) constant 1
log P

Chemical Potentials

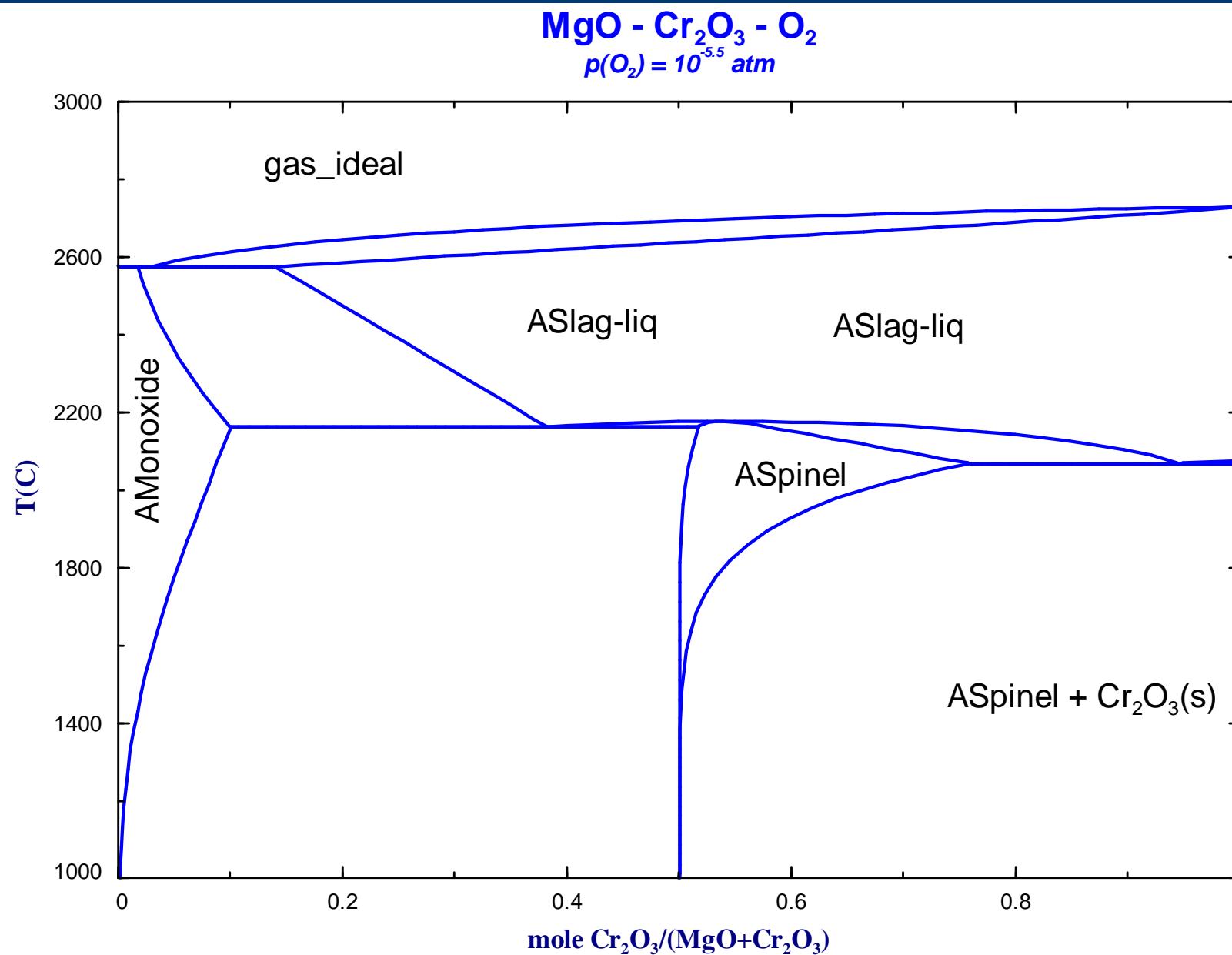
#1. log10(p) = constant
O₂ gas-FACT53 -5.5

Compositions (mole)

#1. $\frac{0 \text{ MgO} + 1 \text{ Cr}_2\text{O}_3}{1 \text{ MgO} + 1 \text{ Cr}_2\text{O}_3} = \frac{\text{X-axis}}{1 (\text{max}) / 0 (\text{min})}$

Cancel OK

MgO-Cr₂O₃ System at $P(O_2)=10^{-5.5}$ atm



MgO-Cr₂O₃ System at $P(O_2)=10^{-5.5}$ atm

F Menu - Phase Diagram: comments

File Units Parameters Variables Help

T(C) P(atm) Energy(J) Mass(mol) Vol(litre)

Components (3)

MgO + Cr₂O₃ + O₂

Products

Compound species

* + gas	<input checked="" type="radio"/> ideal	<input type="radio"/> real	10
aqueous	0		
pure liquids	0		
* + pure solids	2		
<input type="checkbox"/> suppress duplicates	<input type="button" value="apply"/>		

* - custom selection
species: 12

Target
- none -
Estimate T(K): 1000
Mass(mol): 0

Solution species

*	+	Base-Phase	Full Name
I		FToxic-SLAGA	ASlag-liq
+		FToxic-SPINA	ASpinel
+		FToxic-MeO_A	AMonoxide

Legend
I - immiscible 1
+ - selected 2

Show all selected
species: 17
solutions: 4

Variables

T(C)	log10(p(O ₂))	Cr ₂ O ₃ /(MgO+Cr ₂ O ₃)		
1000 3000	-5.5	0.1		

T(C) vs Cr₂O₃/(MgO+Cr₂O₃)

FactSage 6.2 beta C:\...\PhasCr-Mg-O_MgO-Cr₂O₃-O₂_P(O₂)_gas-metastable.DAT

F Selection - Equilib

File Edit Show Sort

Selected: 10/10 GAS Sorted by Code

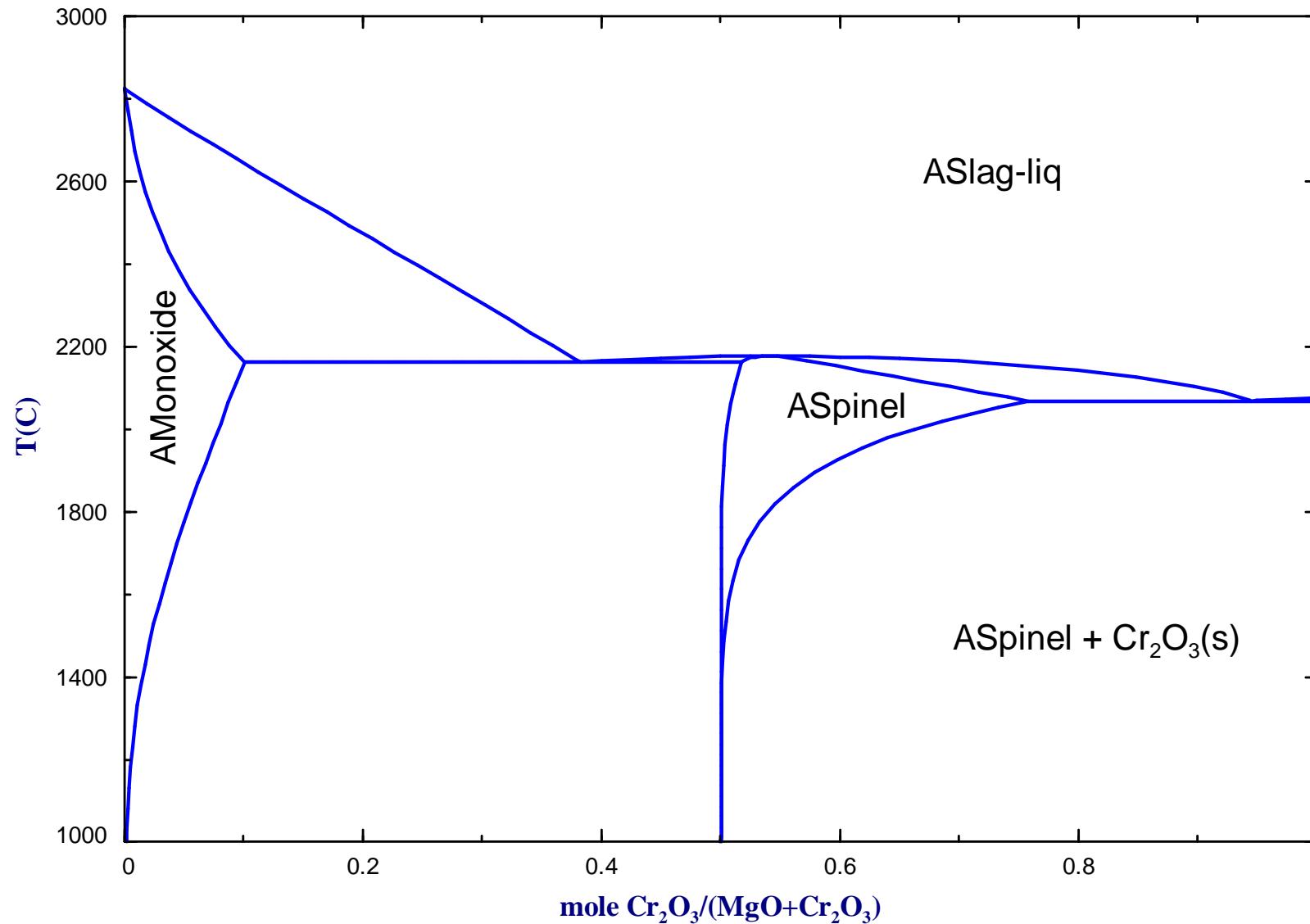
+	Code	Species	Data	Phase	T	V	Activity
!	1	O(g)	FACT53	gas			
!	2	O ₂ (g)	FACT53	gas			
!	3	O ₃ (g)	FACT53	gas			
!	4	Mg(g)	FACT53	gas			
!	5	Mg ₂ (g)	FACT53	gas			
!	6	MgO(g)	FACT53	gas			
!	7	Cr(g)	FACT53	gas			
!	8	CrO(g)	FACT53	gas			
!	9	CrO ₂ (g)	FACT53	gas			
!	10	CrO ₃ (g)	FACT53	gas			

Show Selected Select All Select/Clear... Clear OK

**Gas phase must be selected,
but it can be made dormant**

MgO-Cr₂O₃ System at $P(O_2)=10^{-5.5}$ atm, Dormant Gas

MgO - Cr₂O₃ - O₂
 $p(O_2) = 10^{-5.5}$ atm



Fe-Cr-O System at 1300 °C

F Components - Phase Diagram

File Edit Units Data Search Help

T(C) P(atm) Energy(J) Mass(mol) Vol(litre)

Components

Fe
Cr
O₂

Data Search

Databases - 3/24 compound databases, 2/22 solution databases

Fact

ELEM
 FACT
 Fact53
 FTToxic
 FTsalt
 FTmisc
 FTball
 FThelg
 FTpulp
 FTlite

FactSage™

FSopp
 FSlead
 FSelite
 FSstel
 FSups
 FSnobl

SGTE

BINS
 SGPS
 SGTE
 SGnobl
 SGsold
 SGnucl

compounds only
solutions only
no data

Miscellaneous

EXAM
 SGSL
 SGTE*

Clear All
Select All
Add/Remove Data
RefreshDatabases

Information -

Oxide phases

Metal phases from FSstel

Options

Include -
 gaseous ions
 (plasmas)
 aqueous species
 limited data compounds (25C)

Limits -
Organic species CxHy... X(max) =
Minimum solution components: 1 2 cpts

Cancel Summary ... OK

Next >>

FactSage 6.2 beta Compound: 3/24 databases Solution: 2/22 databases

Fe-Cr-O System at 1300 °C

F Menu - Phase Diagram: last system

File Units Parameters Variables Help

T(C) P(atm) Energy(J) Mass(mol) Vol(litre)

Components (3) Fe + Cr + O₂

Products

Compound species

- gas ideal real 0
- aqueous 0
- pure liquids 0
- * pure solids 5
- suppress duplicates

* - custom selection species: 5

Target - none -

Estimate T(K): 1000

Mass(mol): 0

Solution species

*	Base-Phase	Full Name
+	FSstel-FCC	FCC_A1:Me(C,N)
+	FSstel-BCC	BCC_A2
+	FSstel-SIGM	SIGMA
+	FSstel-FE-L	Fe-LIQUID
I	FToxic-SLAGA	ASlag-liq
+	FToxic-SPINA	ASpinel
+	FToxic-MeO_A	AMonoxide
+	FToxic-CORU	M2O3(Corundum)

Legend
I- immiscible 1
+ - selected 7

Show all selected
species: 40
solutions: 9

Variables

T(C)	log10(p(O ₂))	Cr/(Fe+Cr)		
1300	-20.0	0.1		

log10(p(O₂)) (atm) vs Cr/(Fe+Cr)

FactSage 6.2 beta C:\...\PhasCr-Fe-O_1300C_Variable-P(O2).DAT

Oxide phases

Nothing from Fact53 and from FSstel



F Selection - Equilib

File Edit Show Sort

Selected: 5/31 Duplicates selected. SOLID Sorted by Code

+	Code	Species	Data	Phase	T	V	Activity
36	Fe ₃ O ₄ (s)	FACT53	magnetite		V		
37	Fe ₃ O ₄ (s2)	FACT53	magnetite		V		
38	Fe ₃ O ₄ (s3)	FACT53	high-pressure...		V		
39	Fe ₃ O ₄ (s4)	FACT53	high-pressure...		V		
40	FeCr ₂ O ₄ (s)	FACT53	solid				
41	Cr(s)	FSstel	bcc_a2				
42	Cr ₂ O ₃ (s)	FSstel	solid				
43	Fe(s)	FSstel	bcc_a2				
44	Fe(s2)	FSstel	fcc_a1				
45	Fe ₂ O ₃ (s)	FSstel	hematite		V		
46	Fe ₃ O ₄ (s)	FSstel	magnetite		V		
47	Fe ₃ O ₄ (s2)	FSstel	magnetite		V		
48	FeCr ₂ O ₄ (s)	FSstel	solid				
49	Cr ₂ O ₃ (s)	FToxid	solid				
50	Cr ₃ O ₄ (s)	FToxid	solid		o		
51	Fe ₂ O ₃ (s)	FToxid	hematite		V		
52	Fe ₂ O ₃ (s2)	FToxid	high-pressure...		V		
53	Fe ₂ O ₃ (s3)	FToxid	high-pressure...		V		

Now Selected Select All Select/Clear... Clear OK

Fe-Cr-O System at 1300 °C

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

Variables

Y (radio button selected)
X
A
B
C
compositions 1
log10(a) 1
Y steps: 5
X steps: 5
Next >>

T and P

Temperature: T(C) constant 1300
Pressure: P(atm) constant 1
log P

Chemical Potentials

#1. log10(p) = Y-axis
O₂ 0
gas-FACT53 -20

Compositions (mole)

#1. $\frac{0 \text{ Fe} + 1 \text{ Cr}}{1 \text{ Fe} + 1 \text{ Cr}} = X\text{-axis}$
1 (max)
0 (min)

Cancel OK

Fe-Cr-O System at 1300 °C

