

The *Predom* module

Use *Predom* to calculate and plot isothermal 1-, 2- and 3-metal predominance area diagrams.

Predom makes exclusively use of compound databases.

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NOTE: Use the HOME/Pos1 button to return to the table of contents.

The *Predom* module



Click on *Predom* in the main *FactSage* window.

The *Predom* methodology

The following series of three slides shows how the **phase boundaries** in a **predominance area type diagram** are related to the **coefficients** defined by a **stoichiometric reaction**.

The **Gibbs energy minimum principle** is obeyed at all points of the diagram.

Using the **Reaction** program to identify the most probable reaction

Question: A gas mixture, 80% SO_2 + 20% O_2 at 1 atm, is equilibrated with Fe at 1000 K. What are the stable products?

Answer: Although some $\text{SO}_3(\text{g})$ forms, for simplicity we will assume that SO_2 and O_2 are at equilibrium: i.e., $P_{\text{SO}_2} = 0.8 \text{ atm}$ and $P_{\text{O}_2} = 0.2 \text{ atm}$. In such a case, it can be shown that the equilibrium partial pressure of sulfur is $P_{\text{S}_2} = 10^{-29} \text{ atm}$. Although the value is small, this chemical potential is useful for thermodynamic calculations.

From the **Reaction** program, the following values of ΔG are calculated:
(note: 1 mol Fe(s) reactant in all cases)

1 : Fe(s) + 0.5 O ₂ (0.2 atm) = FeO	$\Delta G = -193.2 \text{ kJ}$
2 : Fe(s) + 0.75 O ₂ (0.2 atm) = 0.5 Fe ₂ O ₃	$\Delta G = -271.5 \text{ kJ}$
3 : Fe(s) + (2/3) O ₂ (0.2 atm) = (1/3) Fe ₃ O ₄	$\Delta G = -254.7 \text{ kJ}$
4 : Fe(s) + 0.5 S ₂ (10 ⁻²⁹ atm) = FeS	$\Delta G = 181.6 \text{ kJ}$
5 : Fe(s) + S ₂ (10 ⁻²⁹ atm) = FeS ₂	$\Delta G = 454.2 \text{ kJ}$
6 : Fe(s) + 2 O ₂ (0.2 atm) + S ₂ (10 ⁻²⁹ atm) = FeSO ₄	$\Delta G = -266.1 \text{ kJ}$
7 : Fe(s) + 3 O ₂ (0.2 atm) + 0.75 S ₂ (10 ⁻²⁹ atm) = 0.5 Fe ₂ (SO ₄) ₃	$\Delta G = -279.2 \text{ kJ}$

Reaction program: 7 possible isothermal isobaric reactions and 7 values of ΔG

F Reactants - Reaction

File Edit Units Data Search Help

T(K) P(atm) Energy(J) Mass(mol) Vol(l)

1-3

Mass(mol)	Species	Phase	T(K)	P(atm)**	Activity	Data
1	Fe	most stable	1000	1.0	1.0	FACT
+ 0.5	O2	gas	1000	0.2		FACT
= 1	FeO	most stable	1000	1.0		FACT

*** For a gas species, P(atm/bar/...
For a liquid or solid, P is the hydro...
- molar volume (but not compressibility)

non standard states

Next

FactSage 5.1 Compound: FACT ELEM SGPS SGSL

Reaction 1

F Table Reaction

File Units Output Figure Help

T(K) P(atm) Energy(J) Mass(mol) Vol(l)

Reactants

$$\text{Fe (1000K)} + 0.5 \text{ O}_2 \text{ (1000K, 0.2atm,g)} = \text{FeO (1000K)}$$

Delta H(J)	Delta G(J)	Delta Vol(l)	Delta S(J/K)	Delta Cp(J/K)	Delta A (J)	T
-----	Fe(s1)	O2(g)	FeO(s)	-----		
-263477.5	-193172.6	-2.0514E+02	-70.305	-14.006	-193709.3	

Reaction 2

Reactants

$$\text{Fe (1000K)} + 0.75 \text{ O}_2 \text{ (1000K, 0.2atm,g)} = 0.5 \text{ Fe}_2\text{O}_3 \text{ (1000K)}$$

Delta H(J)	Delta G(J)	Delta Vol(l)	Delta S(J/K)	Delta Cp(J/K)	Delta A (J)	T
-----	Fe(s1)	O2(g)	Fe2O3(s1)	-----		
-403975.4	-271480.7	-3.0771E+02	-132.495	-5.638	-268340.6	

Reaction 3

Reactants

$$\text{Fe (1000K)} + 0.6667 \text{ O}_2 \text{ (1000K, 0.2atm,g)} = 0.3333 \text{ Fe}_3\text{O}_4 \text{ (1000K)}$$

Delta H(J)	Delta G(J)	Delta Vol(l)	Delta S(J/K)	Delta Cp(J/K)	Delta A (J)	T
-----	Fe(s1)	O2(g)	Fe3O4(s2)	-----		
-363290.8	-254702.5	-2.7353E+02	-108.588	-10.220	-253853.4	

Predom methodology

Reaction
4

Reactants						
Fe + 0.5 S2 = FeS (1000K) (1000K,1E-29atm,g) (1000K)						
Delta H(J)	Delta G(J)	Delta Vol(l)	Delta S(J/K)	Delta Cp(J/K)	Delta A (J)	T
-----	Fe(s1)	S2(g)	FeS(s3)	-----		
-153754.8	181584.6	-4.1029E+30	-335.339	-13.741	181047.4	

Reaction
5

Reactants						
Fe + S2 = FeS2 (1000K) (1000K,1E-29atm,g) (1000K)						
Delta H(J)	Delta G(J)	Delta Vol(l)	Delta S(J/K)	Delta Cp(J/K)	Delta A (J)	T
-----	Fe(s1)	S2(g)	FeS2(s1)	-----		
-297458.5	454223.7	-8.2058E+30	-751.682	-8.904	457843.1	

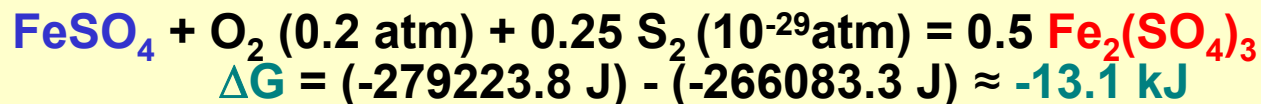
Reaction
6

Reactants						
Fe + 2 O2 + 0.5 S2 = FeSO4 (1000K) (1000K,0.2atm,g) (1000K,1E-29atm,g) (1000K)						
Delta H(J)	Delta G(J)	Delta Vol(l)	Delta S(J/K)	Delta Cp(J/K)	Delta A (J)	T
-----	Fe(s1)	O2(g)	S2(g)	FeSO4(s)	-----	
-979627.1	-266083.3	-4.1029E+30	-713.544	13.040	-249989.6	

Reaction
7

Reactants						
Fe + 3 O2 + 0.75 S2 = 0.5 Fe2(SO4)3 (1000K) (1000K,0.2atm,g) (1000K,1E-29atm,g) (1000K)						
Delta H(J)	Delta G(J)	Delta Vol(l)	Delta S(J/K)	Delta Cp(J/K)	Delta A (J)	T
-----	Fe(s1)	O2(g)	S2(g)	Fe2(SO4)3(s)	-----	
-1373001.6	-279223.8	-6.1543E+30	-1093.778	17.991	-252743.6	

$\text{Fe}_2(\text{SO}_4)_3$ is the stable product since ΔG is the most negative. For example, FeSO_4 could not be the most stable since combining reactions 6 and 7, we have:



This methodology is used by the *Predom* program to locate the domains of stability of each phase as a function of gas potential.

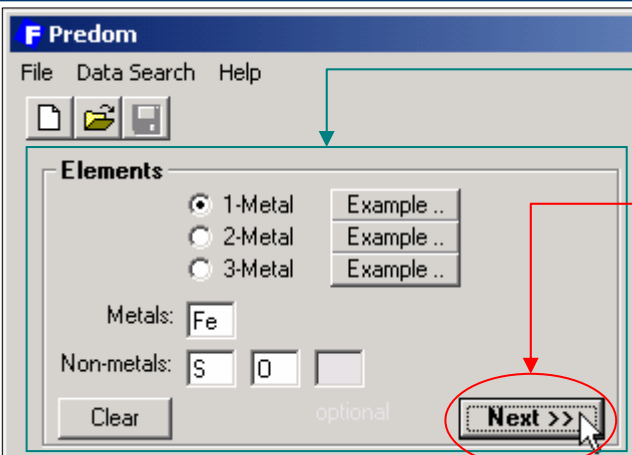
Specifying a **classical predominance** area diagram

The system **Fe-S₂-O₂** for **T=1000K** and a total **pressure** of **1 atm** is used as an example case for a classical predominance area type diagram.

In the following two slides the input for the **definition** of the diagram and its **axes variables** as well as the calculated diagram are shown.

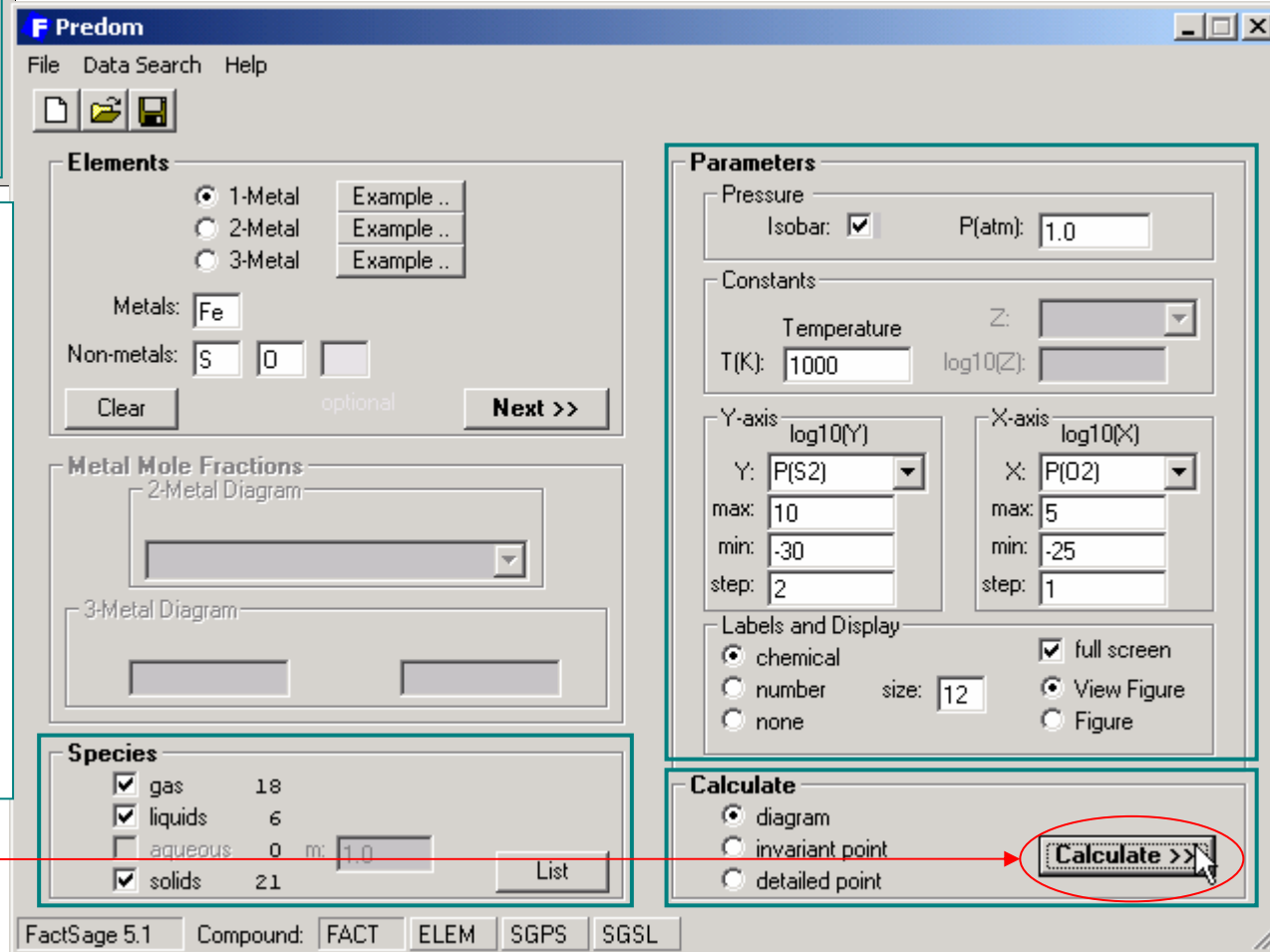
The diagram is displayed using the ***View Figure*** module.

Specifying a classical predominance area diagram: $\text{Fe-S}_2(\text{g})\text{-O}_2(\text{g})$ at 1000 K



1. Specify the metallic and the non-metallic elements.

2. Press **Next >>** to activate the calculation.



3. Select the variables:

• Parameters:

- Pressure
- Constants
- Axes
- Labels and Display

• Species: gas, liquids and solids

• Calculate: a diagram

4. Press **Calculate >>**

View Figure display of a predominance area diagram

Although the **View Figure** diagram is crude and can not be edited, it is a very efficient module that uses only a small amount of computer memory.

Assumptions:

- all solids are pure
- the total pressure is unconstrained

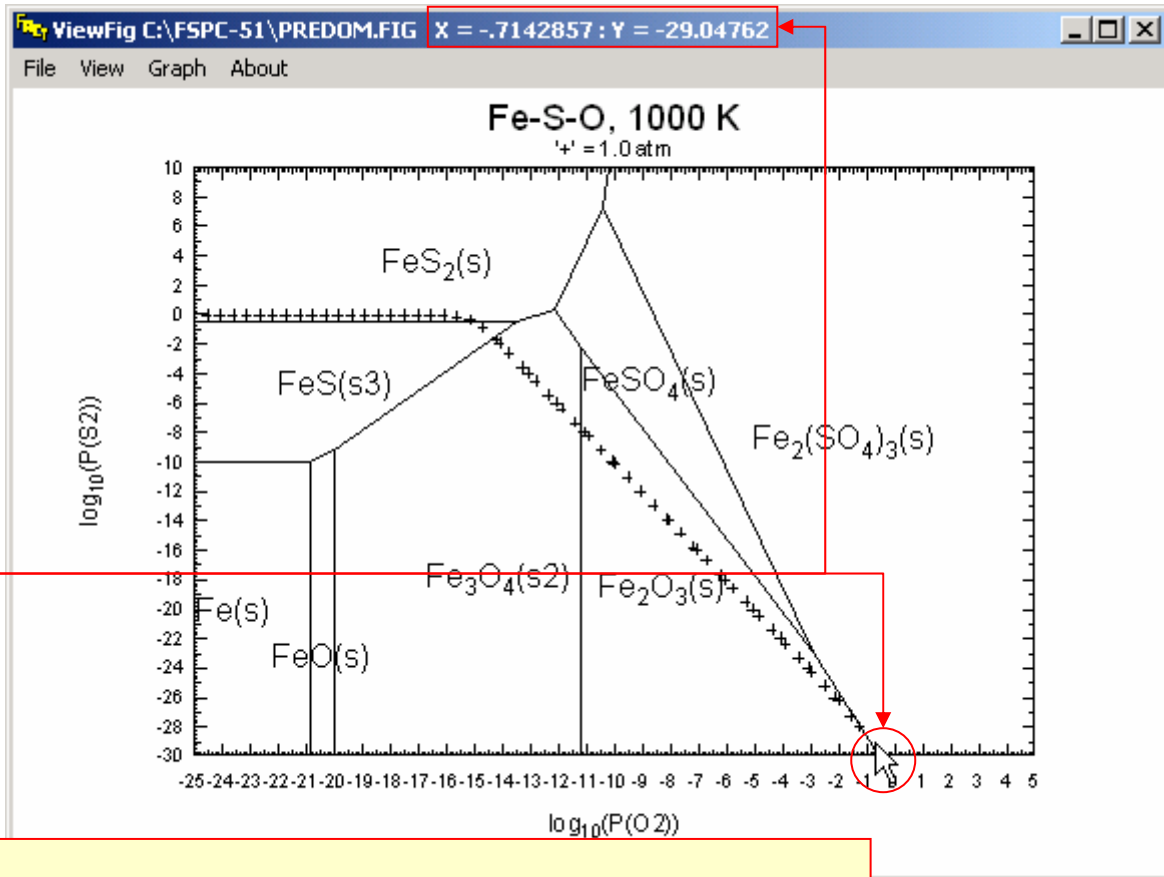
The arrow is pointing to:

$$x = \log_{10} P_{O_2} = -0.7143$$

$$\rightarrow P_{O_2} \approx 0.2 \text{ atm}$$

$$y = \log_{10} P_{S_2} = -29.05$$

$$\rightarrow P_{S_2} \approx 10^{-29} \text{ atm}$$



Observations:

- **Fe₂(SO₄)₃(s)** is the stable product at **P_{S₂}** = 10⁻²⁹ atm and **P_{O₂}** = 0.2 atm
- **Fe** can not coexist with **Fe₃O₄** (they react to form **FeO**)
- **FeS₂** is only stable at high **P_{S₂}** (i.e. very high total pressures)

Displaying the diagram with the *Figure* module

The *Predom* module also permits graphical output using the *Figure* module.

The following two slides show how this is done for a diagram of the $\text{Fe-S}_2\text{-O}_2$ system and one for the $\text{Fe-SO}_2\text{-O}_2$ system.

Figure display of the predominance area diagram of $\text{Fe-S}_2(\text{g})\text{-O}_2(\text{g})$ at 1000 K

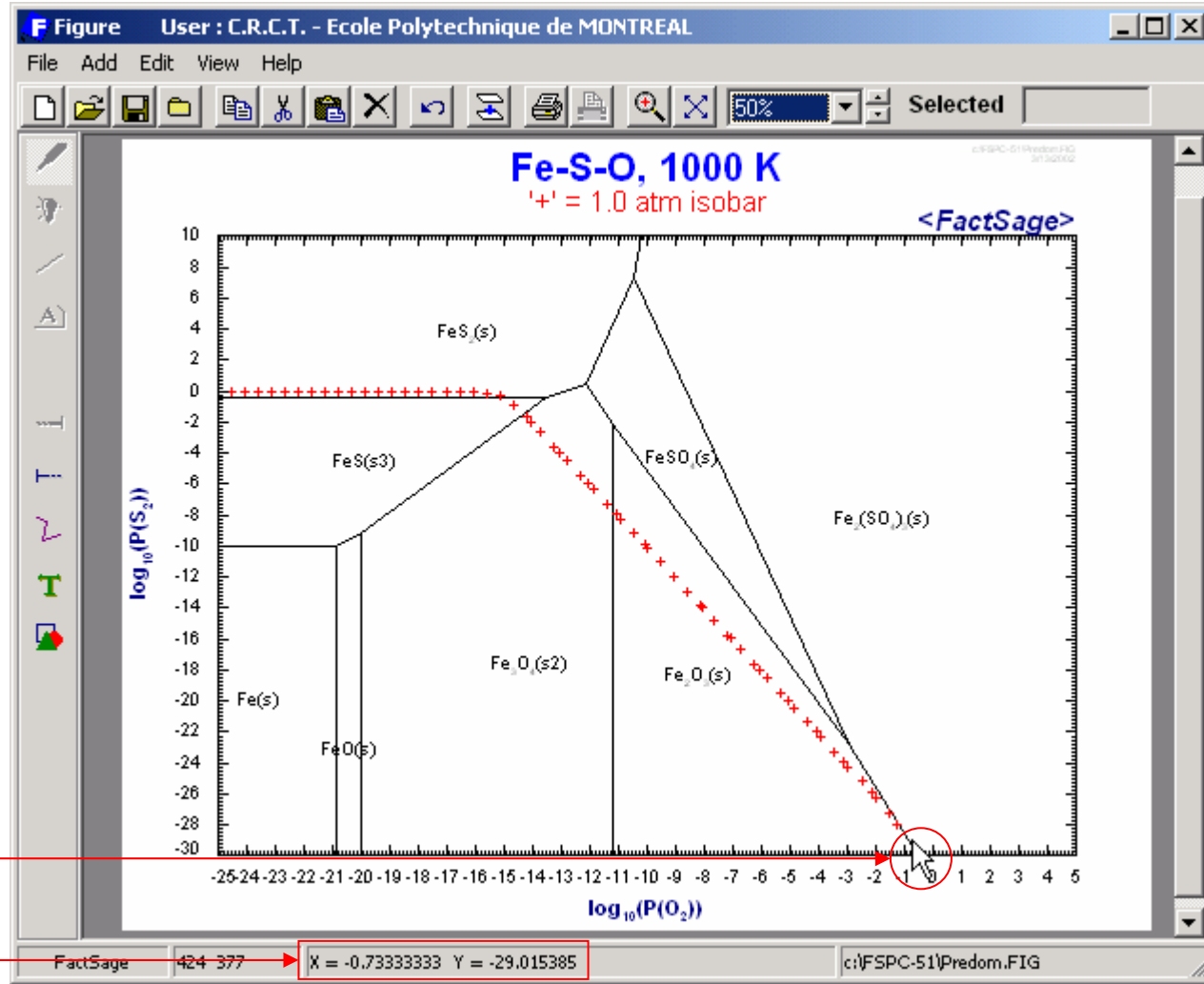
Labels and Display

- chemical
- number size: 12
- none
- full screen
- View Figure
- Figure

Calculate

- diagram
- invariant point
- detailed point

Calculate >>



The arrow is pointing to:

$x = \log_{10} P_{\text{O}_2} = -0.7333$
→ $P_{\text{O}_2} \approx 0.2 \text{ atm}$

$y = \log_{10} P_{\text{S}_2} = -29.01$
→ $P_{\text{S}_2} \approx 10^{-29} \text{ atm}$

Figure creates a predominance diagram that can be edited, manipulated and stored in a variety of ways. This powerful module uses a lot of computer memory.

Revised *Predom* diagram displayed in *Figure* for $\text{Fe-SO}_2(\text{g})\text{-O}_2(\text{g})$ at 1000 K

Changing the X and Y axes.

Parameters

Pressure
Isobar: P(atm): 1.0

Constants
Temperature T(K): 1000
Z: log10(Z):

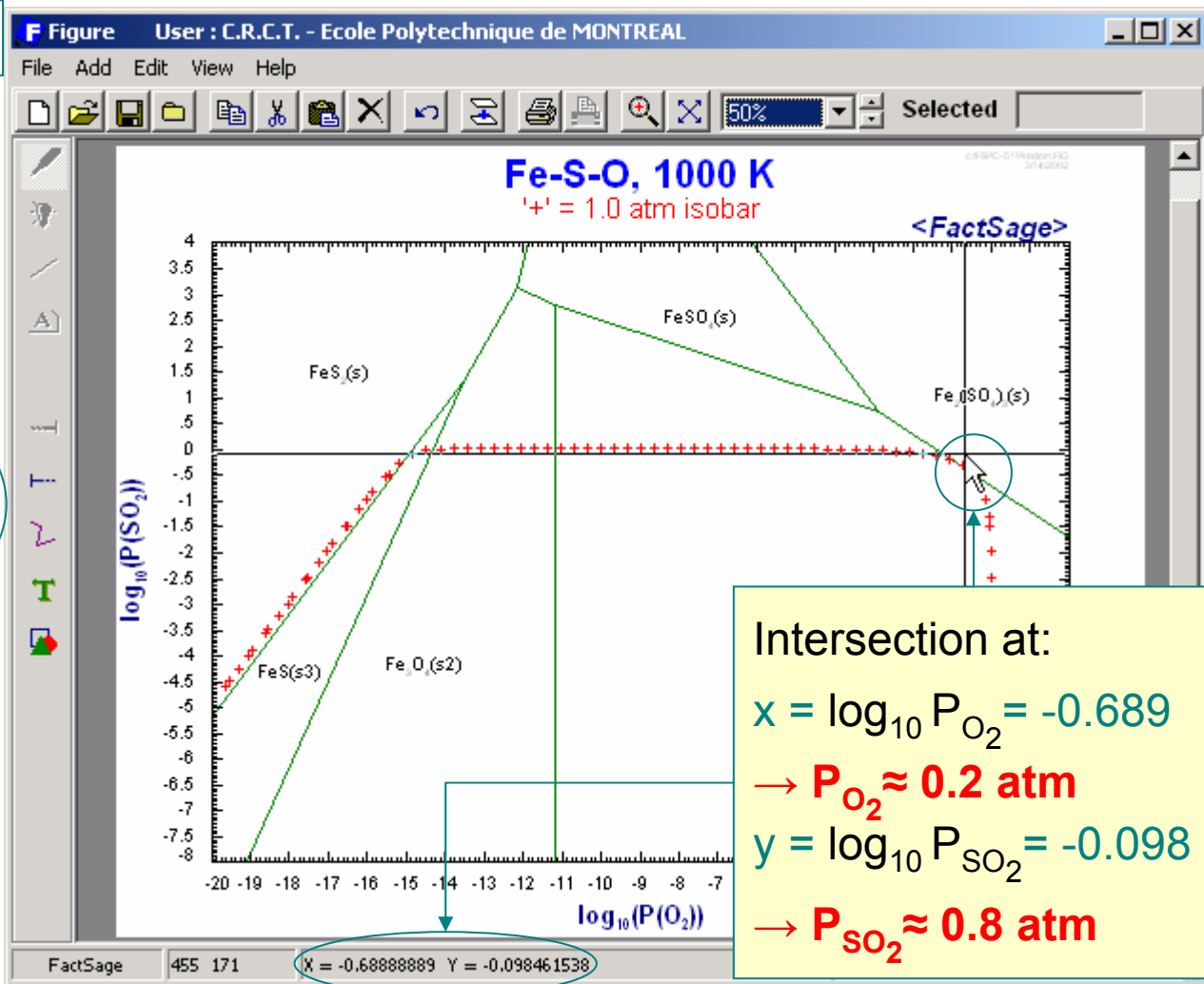
Y-axis log10(Y)
Y: P(SO2) max: 4 min: -8 step: 0.5

X-axis log10(X)
X: P(O2) max: 2 min: -20 step: 1

Labels and Display
 chemical number none size: 12
 full screen View Figure Figure

Calculate
 diagram invariant point detailed point

Calculate >>



And **Calculate >>...**
a revised *Predom* diagram.

Note: The $\text{Fe-S}_2(\text{g})\text{-O}_2(\text{g})$ diagram (previous page) and the $\text{Fe-SO}_2(\text{g})\text{-O}_2(\text{g})$ diagram (here) are topologically equivalent, i.e. the same combination of species coexists at the invariant points.

Numerical results related to the diagrams can be displayed in tabular form.

The following three slides show which **option** boxes need to be **checked** in order to obtain the appropriate output and in which **form** the output is given.

Invariant points of Fe-SO₂(g)-O₂(g) at 1000 K.

Calculate

- diagram
- invariant point
- detailed point

Calculate >>

Phase Rule:

$$F = C - P + 2$$

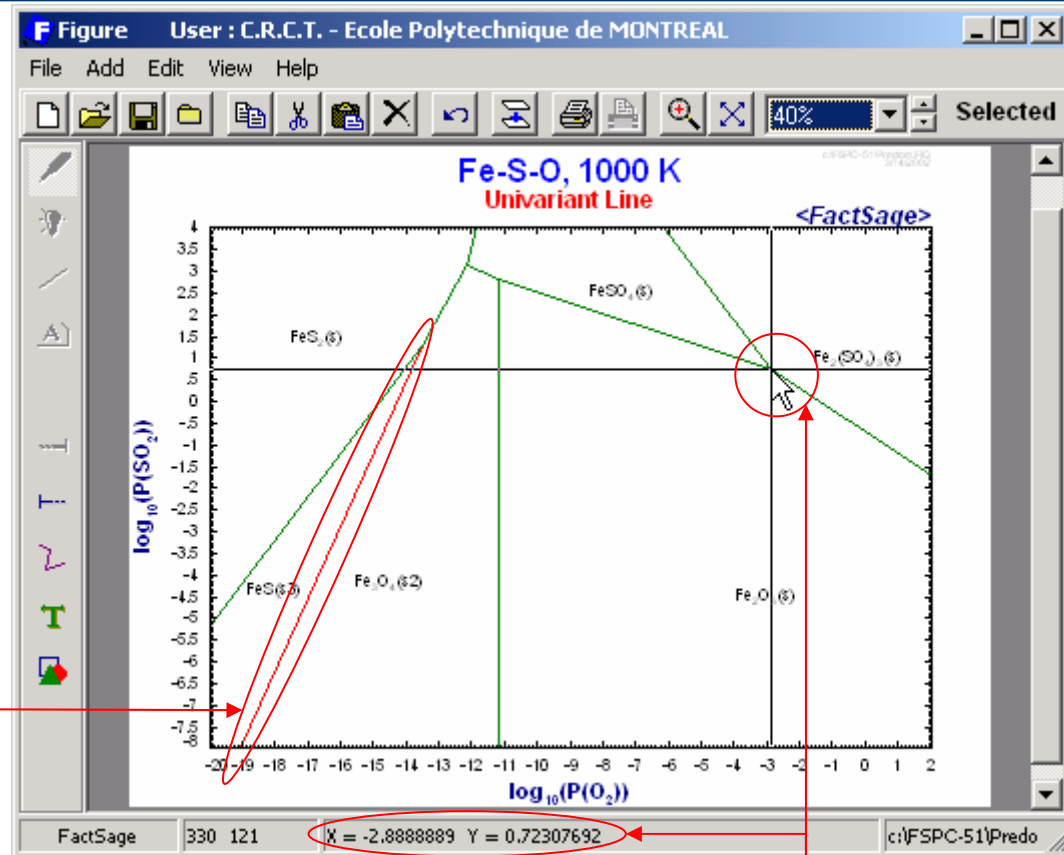
F : degrees of freedom

C : number of components

P : number of phases

Univariant line (l):

FeS/Fe₃O₄/gas. From the phase rule, F = 2. Hence, at 1000 K only one of SO₂ or O₂ can be fixed.



FactSage 330 121 X = -2.8888889 Y = 0.72307692 c:\FSPC-51\Predo

Invariant Points - Y = P(SO₂), X = P(O₂), T = 1000 (K).

log10[Y]	log10[X]		Species		Species		Species
-10.810	-20.879	8	Fe(s)	10	FeO(s)	20	FeS(s3)
-9.491	-19.999	10	FeO(s)	15	Fe3O4(s2)	20	FeS(s3)
2.791	-11.193	11	Fe2O3(s)	15	Fe3O4(s2)	24	FeSO4(s)
0.719	-2.906	11	Fe2O3(s)	24	FeSO4(s)	25	Fe2(SO4)3(s)
1.299	-13.525	15	Fe3O4(s2)	20	FeS(s3)	21	FeS2(s)
3.114	-12.164	15	Fe3O4(s2)	21	FeS2(s)	24	FeSO4(s)
8.261	-10.448	21	FeS2(s)	24	FeSO4(s)	25	Fe2(SO4)3(s)

At the arrow, C = 3 (Fe,S,O) and P = 4 (3 solids and 1 gas); hence F = 1. At 1000 K, the system is invariant. (Note that the total pressure is not specified.)

Detailed point calculation at $P_{\text{SO}_2}=0.8$ atm and $P_{\text{O}_2}=0.2$ atm for $\text{Fe-SO}_2(\text{g})\text{-O}_2(\text{g})$ at 1000K

18 gas species, 6 liquid species and 21 solids species (total: 46 species) in the **FACT** compound database containing **Fe, S** and/or **O**.

Parameters

Pressure
Isobar: P(atm): 1.0

Constants
Temperature: 1000 Z:
T(K): 1000 log10(Z):

Y-axis: log10(Y) X-axis: log10(X)
Y: P(SO2) X: P(O2)
max: 4 max: 2
min: -8 min: -20
step: 0.5 step: 1

Labels and Display
 chemical full screen
 number size: 12 View Figure
 none Figure

Calculate
 diagram
 invariant point
 detailed point

Species
 gas 18
 liquids 6
 aqueous 0 m: 1.0
 solids 21

Compound: FACT ELEM SGPS SGSL

F List - 1000 (K)

+	Code	T	Species	Data	A/P/M	Cp range
Fe gases:						
+	1		Fe(g)	FACT	1.0000E+00	298 - 6000
+	2		FeO(g)	FACT	1.0000E+00	298 - 6000
+	3		FeS(g)	FACT	1.0000E+00	298 - 6000
Fe liquids:						
+	4		Fe(l)	FACT	1.0000E+00	298 - 6000
+	5		FeO(l)	FACT	1.0000E+00	298 - 2000
+	6		Fe3O4(l)	FACT	1.0000E+00	298 - 2500
+	7		FeS(l)	FACT	1.0000E+00	298 - 3800
Fe solids:						
+	8		Fe(s)	FACT	1.0000E+00	298 - 1812
+	9		Fe(s2)	FACT	1.0000E+00	298 - 1812
+	10		FeO(s)	FACT	1.0000E+00	298 - 2000
+	11		Fe2O3(s)	FACT	1.0000E+00	298 - 2500
+	12		Fe2O3(s2)	FACT	1.0000E+00	298 - 1873
+	13		Fe2O3(s3)	FACT	1.0000E+00	956 - 1873
+	14		Fe3O4(s)	FACT	1.0000E+00	298 - 1870

Point Calculation - Y = P(SO2), X = P(O2)
P(SO2): 0.8 Y, X
P(O2): 0.2 log10(Y), log10(X) **Calculate**

Click here (or, from the menu bar, select Data Search > Databases...) to include or exclude a database in the search. Here, only the **FACT** compound database is included.

Point calculation data entry:
 $P_{\text{SO}_2} = 0.8$ atm, $P_{\text{O}_2} = 0.2$ atm

Detailed point calculation at $P_{\text{SO}_2}=0.8$ atm and $P_{\text{O}_2}=0.2$ atm for $\text{Fe-SO}_2(\text{g})\text{-O}_2(\text{g})$ at 1000K

$\text{Fe}_2(\text{SO}_4)_3(\text{s})$ is the stable species:
unit activity, C_p values not extrapolated

A/P/M: Activity/Partial pressure/Molality

F List - Fe-S-O, T = 1000 (K)

Code	T	Species	Data	A/P/M	Cp range
Fe gases:					
1		Fe(g)	FACT	5.137E-29	298 - 6000
2		FeO(g)	FACT	3.004E-23	298 - 6000
3		FeS(g)	FACT	2.528E-40	298 - 6000
Fe liquids:					
4		Fe(l)	FACT	1.144E-15	298 - 6000
5		FeO(l)	FACT	6.901E-06	298 - 2000
6		Fe3O4(l)	FACT	5.325E-08	298 - 2500
7		FeS(l)	FACT	2.396E-25	298 - 3800
Fe solids:					
8		Fe(s)	FACT	2.440E-15	298 - 1812
9		Fe(s2)	FACT	2.343E-15	298 - 1812
10		FeO(s)	FACT	3.001E-05	298 - 2000
11		Fe2O3(s)	FACT	1.370E-01	298 - 2500
12		Fe2O3(s2)	FACT	1.388E-05	298 - 1873
13		Fe2O3(s3)	FACT	1.398E-05	956 - 1873
14		Fe3O4(s)	FACT	1.167E-04	298 - 1870

Total pressure in gas phase = 1.651E+00 atm.

Domain: Fe2(SO4)3(s)

Point Calculation - Y = P(SO2), X = P(O2)

P(SO2): 0.8 Y, X

P(O2): 0.2 log10(Y), log10(X) Calculate

Code	T	Species	Data	A/P/M	Cp range
15		Fe3O4(s2)	FACT	1.207E-04	848 - 2500
16		Fe3O4(s3)	FACT	5.554E-12	298 - 1870
17		Fe3O4(s4)	FACT	5.743E-12	848 - 2500
18		FeS(s)	FACT	6.961E-25	298 - 1400
19		FeS(s2)	FACT	1.144E-15	298 - 6000
20		FeS(s3)	FACT	1.144E-15	298 - 6000
21		FeS2(s)	FACT	1.144E-15	298 - 6000
22		FeS2(s2)	FACT	1.144E-15	298 - 6000
23	T	Fe7S8(s)	FACT	< 1.0E-70	295 - 300
24		FeSO4(s)	FACT	2.015E-01	298 - 2000
25		Fe2(SO4)3(s)	FACT	1.000E+00 *	298 - 2000
Other gases:					
26		O(g)	FACT	6.990E-11	298 - 6000
X 27		O2(g)	FACT	2.000E-01	298 - 6000
28		O3(g)	FACT	7.828E-13	298 - 6000
29		S(g)	FACT	2.304E-23	298 - 2300
30		S2(g)	FACT	1.090E-29	298 - 6000
31		S3(g)	FACT	2.870E-45	298 - 6000
32		S4(g)	FACT	2.787E-60	298 - 6000
33		S5(g)	FACT	< 1.0E-70	298 - 6000
34		S6(g)	FACT	< 1.0E-70	298 - 6000
35		S7(g)	FACT	< 1.0E-70	298 - 6000
36		S8(g)	FACT	< 1.0E-70	298 - 6000
37		SO(g)	FACT	3.405E-12	298 - 6000
Y 38		SO2(g)	FACT	8.000E-01	298 - 6000
39		SO3(g)	FACT	6.511E-01	298 - 6000
40		SSO(g)	FACT	1.016E-23	298 - 6000
Other liquids:					
41		S(l)	FACT	1.422E-15	298 - 1500
42	T	SO3(l)	FACT	1.437E-05	298 - 311
Other solids:					
43	T	S(s)	FACT		298 - 801
44	T	S(s2)	FACT	7.627E-16	298 - 801
45	T	SO3(s)	FACT	3.157E-07	298 - 301

«T» indicates extrapolated data

Mainly SO₂ (0.8 atm), O₂ (0.2 atm) and SO₃ (0.65 atm, see code 39).

Predom diagram for $\text{Cu-SO}_2(\text{g})-\text{O}_2(\text{g})$

The following two slides show how a **series** of isothermal one metal two non-metal components is generated and **overlayed** into a single diagram.

The eight necessary steps are described in detailed.

Predom diagram for $\text{Cu-SO}_2(\text{g})\text{-O}_2(\text{g})$ at 1000 K

1. Specify the metallic elements (**Cu**) and the non-metallic elements (**S** and **O**) in the **Elements** frame.

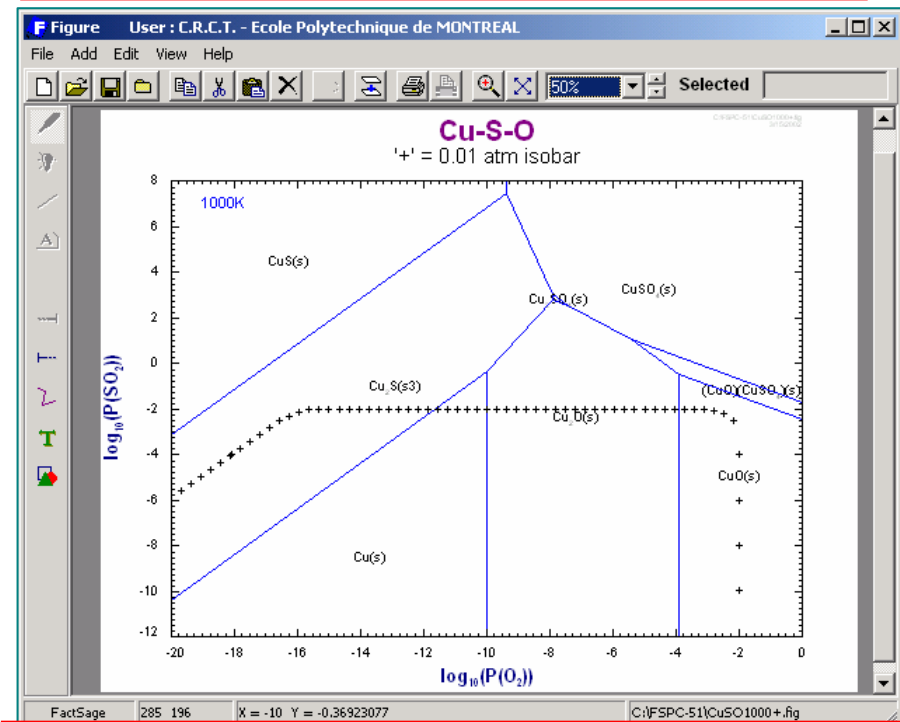
2. Press **Next >>** to search through the selected Compound database(s) (here, **FACT**) and activate the calculation.

3. Specifying an isobar, **P = 0.01 atm**, at **T = 1000 K**.

FactSage 5.1 Compound: FACT ELEM SGPS SGSL

4. Select the **Figure** display and Calculate a **diagram**.

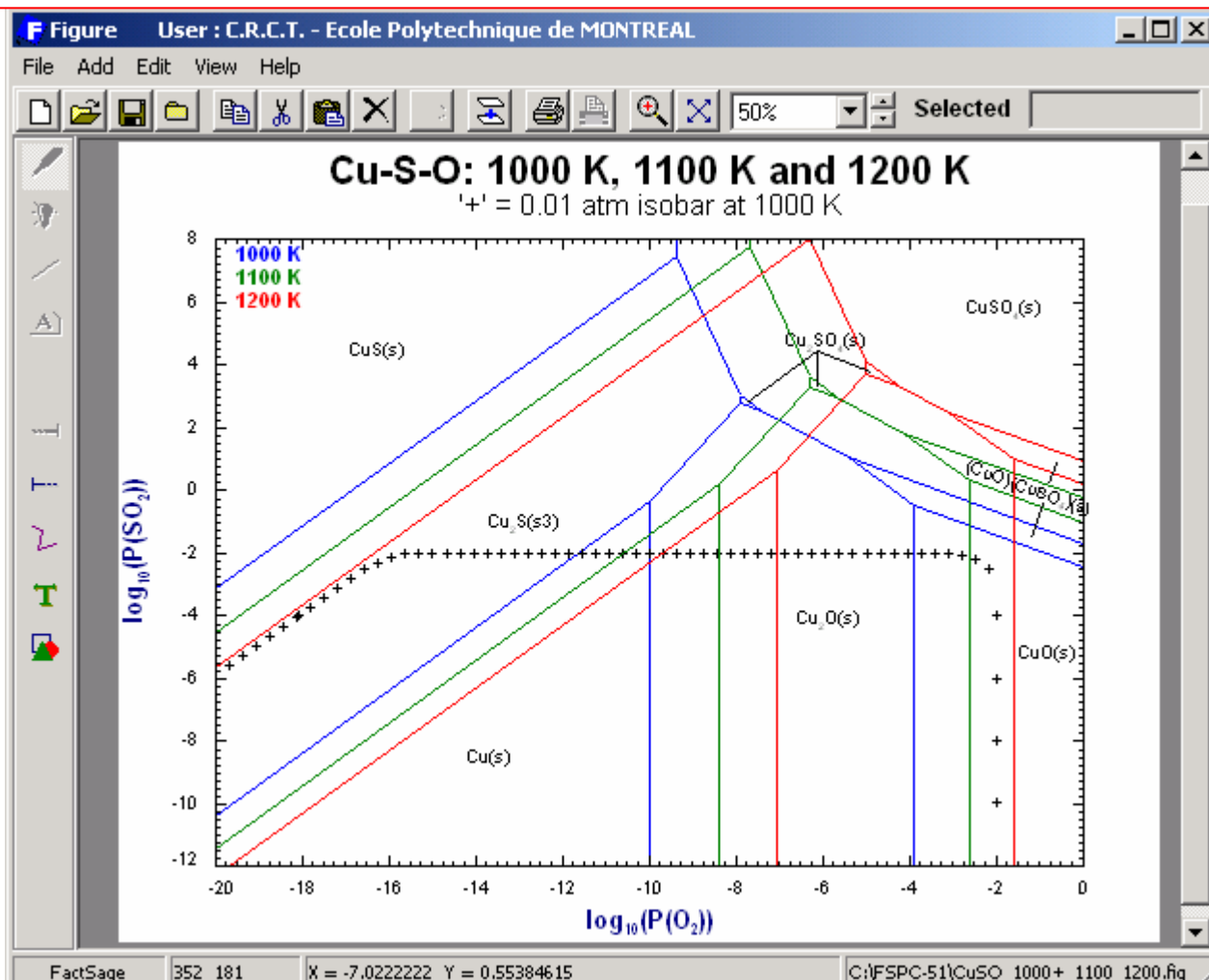
5. Press **Calculate>>**



6. In **Figure**, edit the diagram and save it.

Figure: Superimposed *Predom* diagrams for Cu-SO₂(g)-O₂(g) at 1000, 1100 and 1200 K

7. Repeat steps 3 (but uncheck the isobar checkbox), 5 and 6 for **T=1100 K** and **1200 K**



8. Use the superimpose figure function in the **Figure** program to edit this predominance area diagram at **1000 K**, **1100 K** and **1200 K**.

The following two slides show how a predominance area diagram calculation with **one metal and three non-metal components** is defined and generated.

One-metal predominance diagram with **four elements**: Fe-S-O-Cl

Specifying the isothermal predominance area diagram for:
Fe-S₂(g)-O₂(g)- S₂Cl₂(g) at 1000 K and $P_{S_2Cl_2} = 0.1$ atm

1. Enter the elements. This is a **one-metal Fe** system as metal with **S**, **O** and **Cl** as non-metallic elements.

2. Press **Next >>**.

3. Note: you must enter **2** constants.

- **T = 1000 K**
- **Z = $P_{S_2Cl_2} = 10^{-1}$ atm**

4. Select what you want to calculate and press **Calculate >>**.

The screenshot shows the 'Predom' software interface with the following settings:

- Elements:** 1-Metal selected. Metals: Fe. Non-metals: S, O, Cl. 'Next >>' button is highlighted.
- Parameters:** Pressure: Isobar checked, P(atm): 1.0. Constants: Temperature T(K): 1000, Z: P(CISSCl), log10(Z): -1. Y-axis: log10(Y), Y: P(S2), max: 8, min: -16, step: 2. X-axis: log10(X), X: P(O2), max: 0, min: -20, step: 2.
- Labels and Display:** chemical selected, full screen checked, View Figure unchecked, Figure checked.
- Calculate:** diagram selected, Calculate >> button is highlighted.
- Species:** gas (34), liquids (10), aqueous (0), solids (24). m: 1.0. List button.
- Bottom Bar:** FactSage 5.1, Compound: FACT, ELEM, SGPS, SGSL.

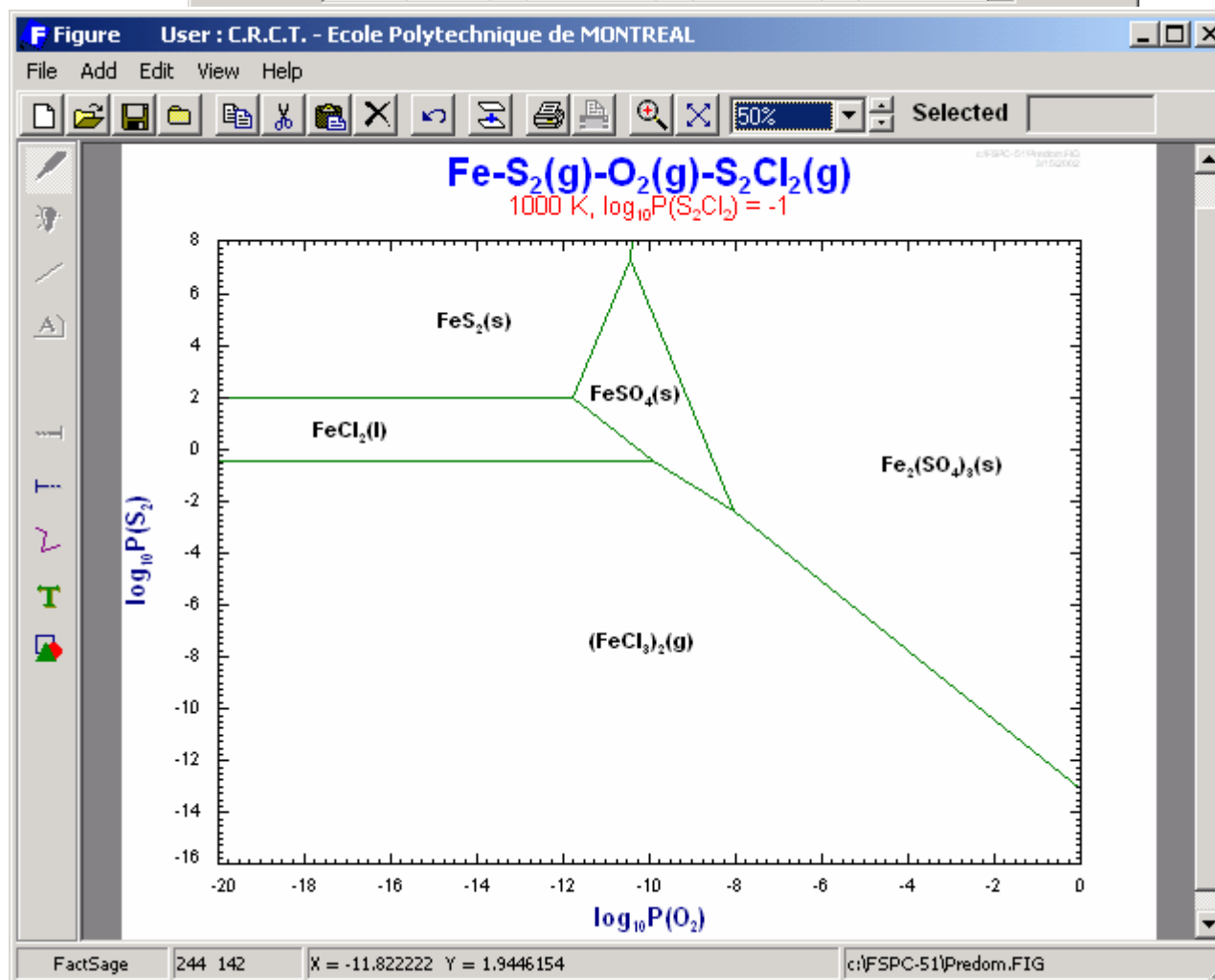
Invariant points table and predominance diagram for Fe-S₂(g)-O₂(g)-S₂Cl₂(g)

Application:
Chlorination of FeS

Invariant Points - Y = P(S₂), X = P(O₂), T = 1000 (K).

log10(Y)	log10(X)		Species		Species		Species
7.251	-10.448	28	FeS ₂ (s)	31	FeSO ₄ (s)	32	Fe ₂ (SO ₄) ₃ (s)
1.940	-11.776	28	FeS ₂ (s)	31	FeSO ₄ (s)	13	FeCl ₂ (l)
-2.424	-8.029	31	FeSO ₄ (s)	32	Fe ₂ (SO ₄) ₃ (s)	8	(FeCl ₃) ₂ (g)
-0.528	-9.925	31	FeSO ₄ (s)	13	FeCl ₂ (l)	8	(FeCl ₃) ₂ (g)

At 1000 K and
 $P_{S_2Cl_2} = 0.1 \text{ atm}$



Various types of **four element predominance** area diagrams

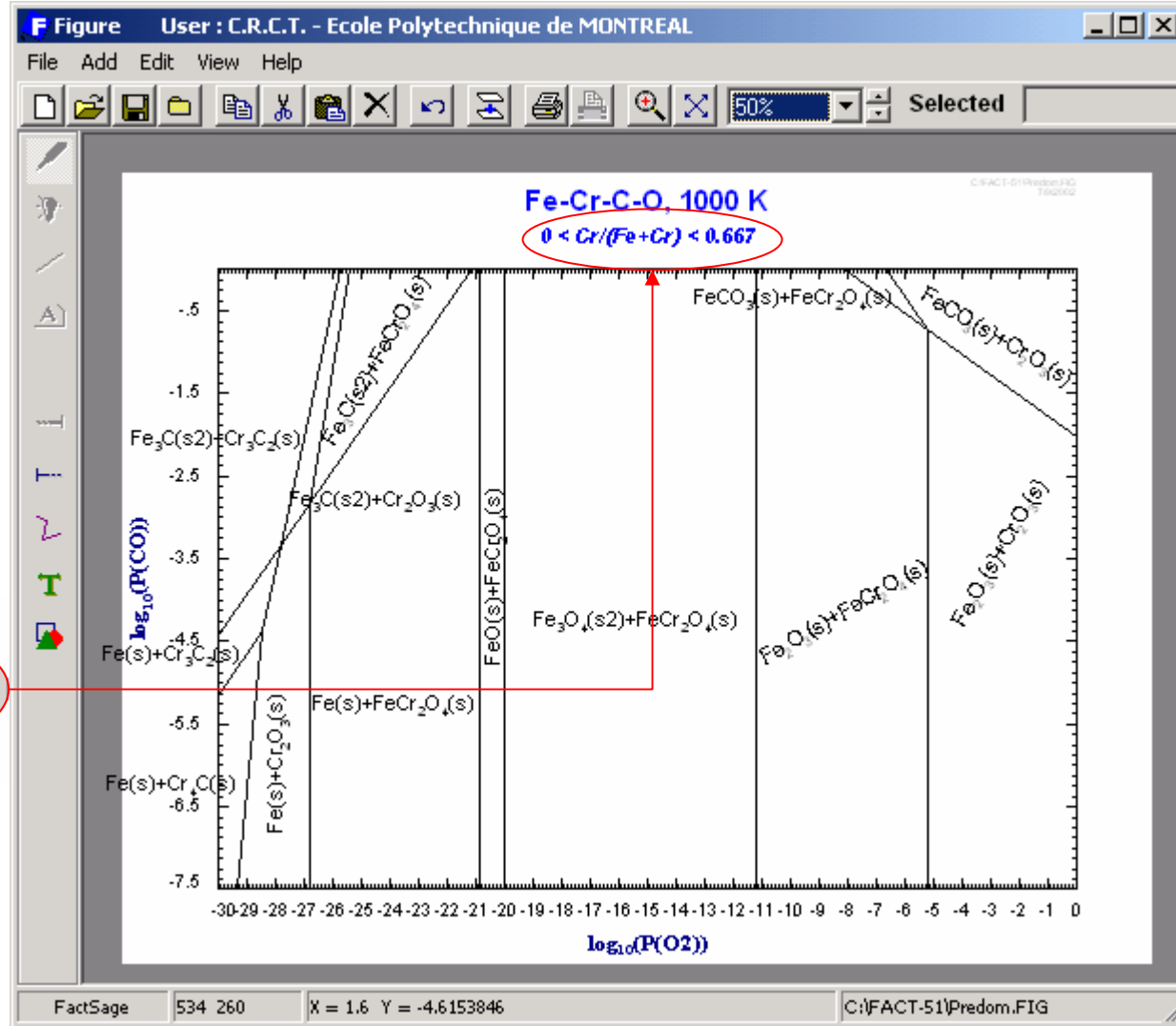
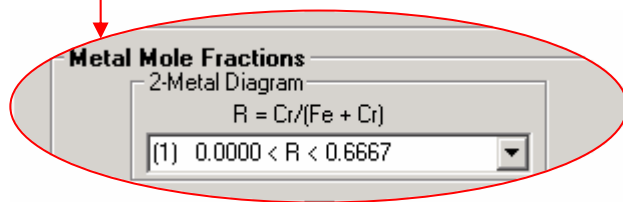
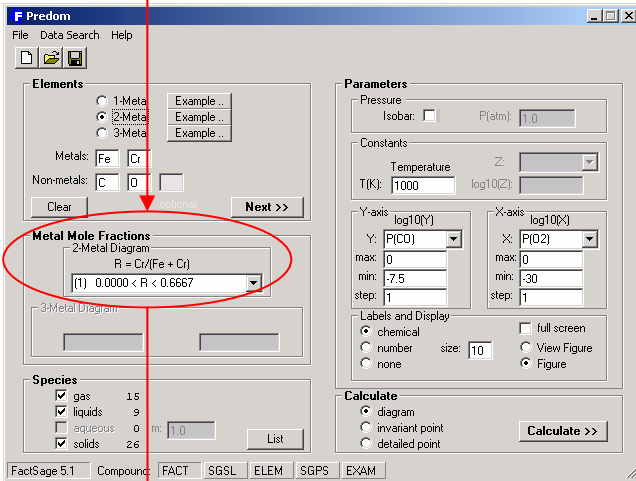
There are **several ways** of generating a predominance area diagram with **two metallic and two non-metallic** elementary components.

The following five slides show how the **Predom** module can be used for the **generation of different types** of four element predominance area diagrams.

Two-metal predominance diagram with **four elements**: Fe-Cr-C-O

Fe-rich side of the iron-chromium two base element predominance area diagram

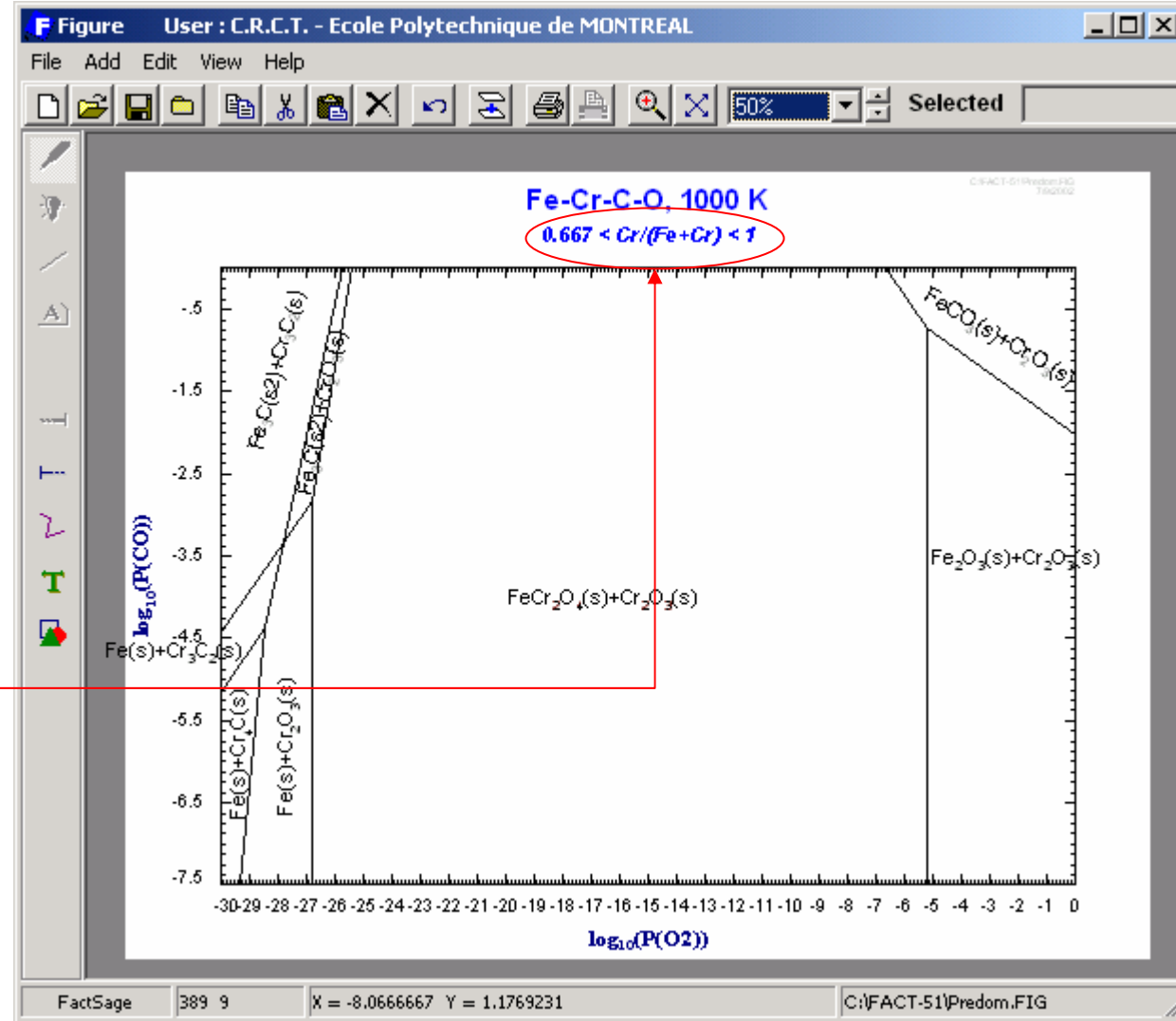
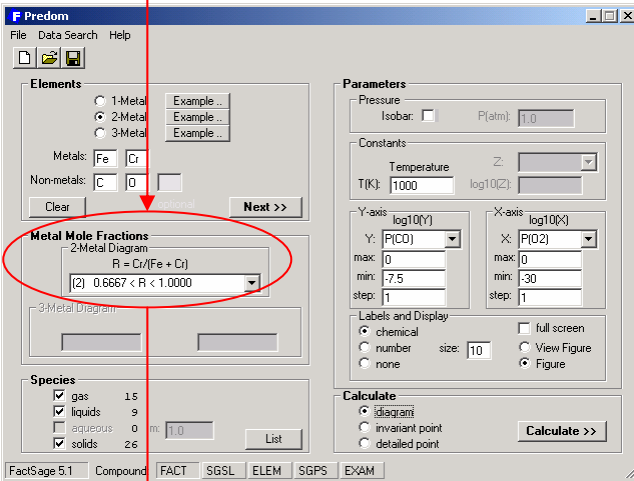
Application:
Passivity of Fe-Cr alloys



Two-metal predominance diagram with **four elements**: Fe-Cr-C-O

Cr-rich side of the iron-chromium two base element predominance area diagram

Application:
Passivity of Fe-Cr alloys



One-metal predominance diagram with **four elements**: Fe-Cr-C-O

Fe-Cr-C-O with Fe as the base element,

$$a_{\text{Cr}(s)} = 1$$

Application:
Passivity of Fe-Cr alloys

Parameters

Pressure: Isobar: P(atm): 1.0

Constants

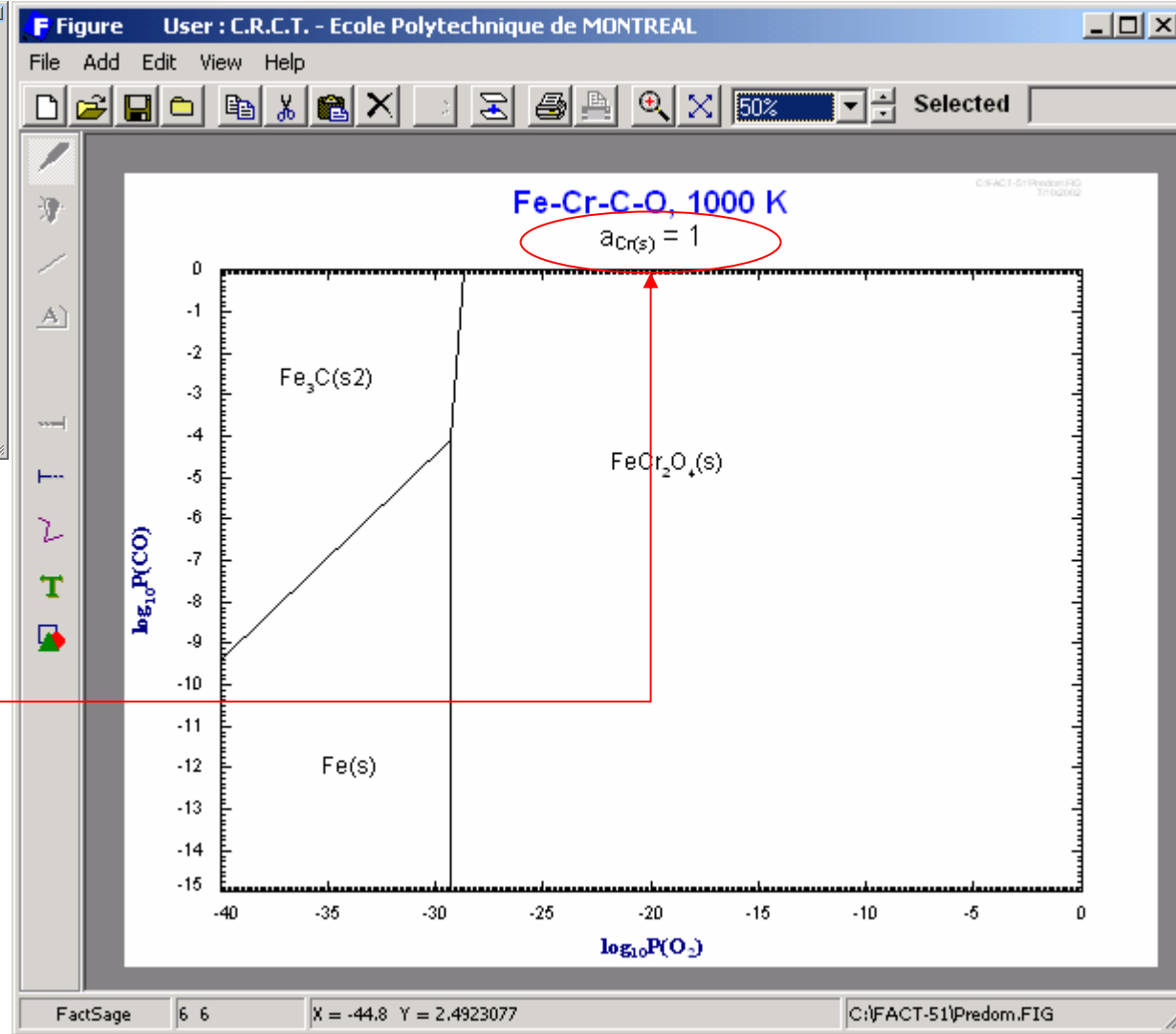
Temperature: 1000 K
log10(Z): 0

Z: a[Cr(s)]

Calculate

diagram
 invariant point
 detailed point

[Calculate >>]



One-metal predominance diagram with **four elements**: Cr-Fe-C-O

Cr-Fe-C-O with Cr as the base element,

$$a_{\text{Fe(s)}} = 1$$

Application:

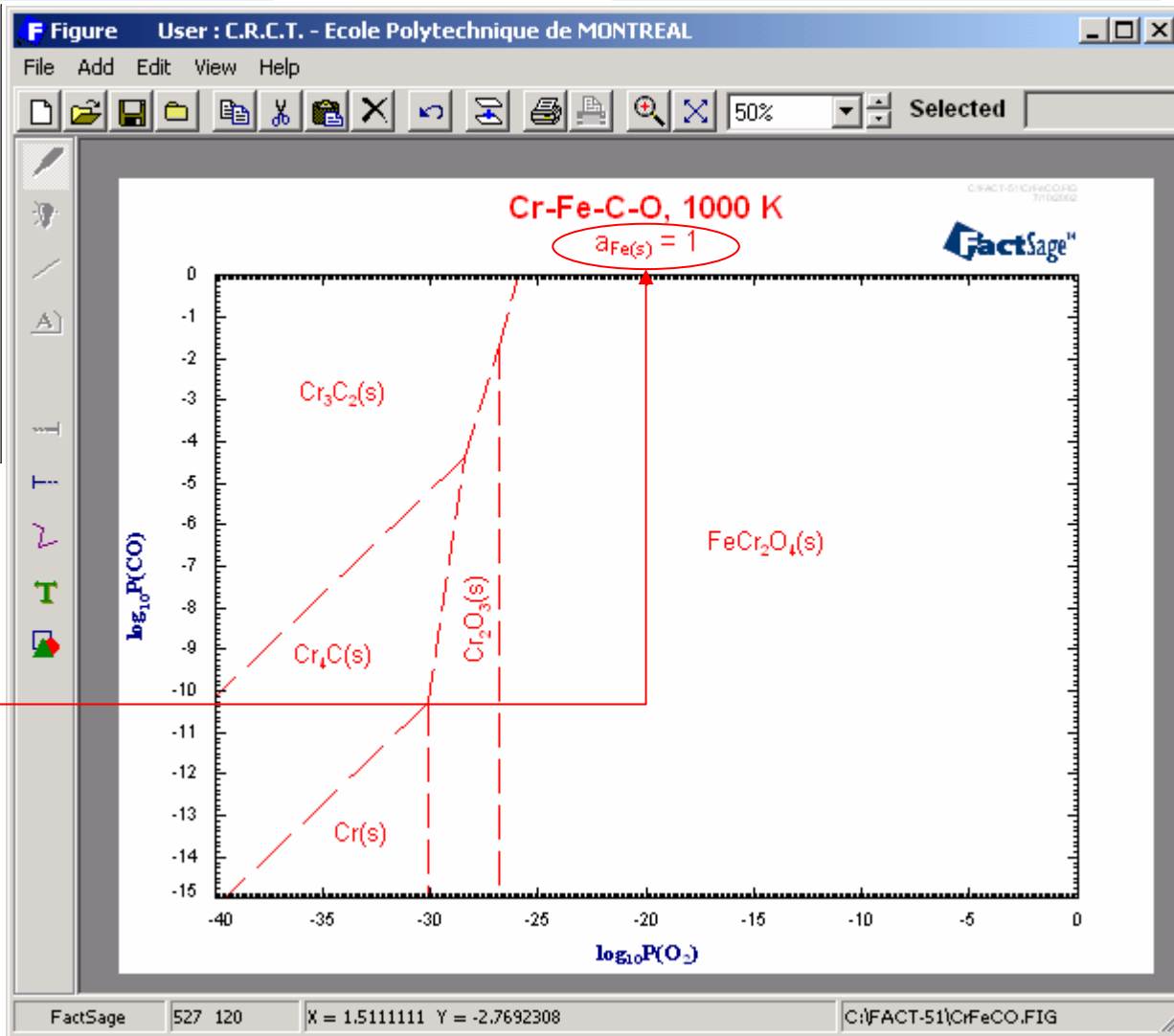
Passivity of Fe-Cr alloys

Predom
File Data Search Help

Elements
Metals: Cr
Non-metals: Fe C O

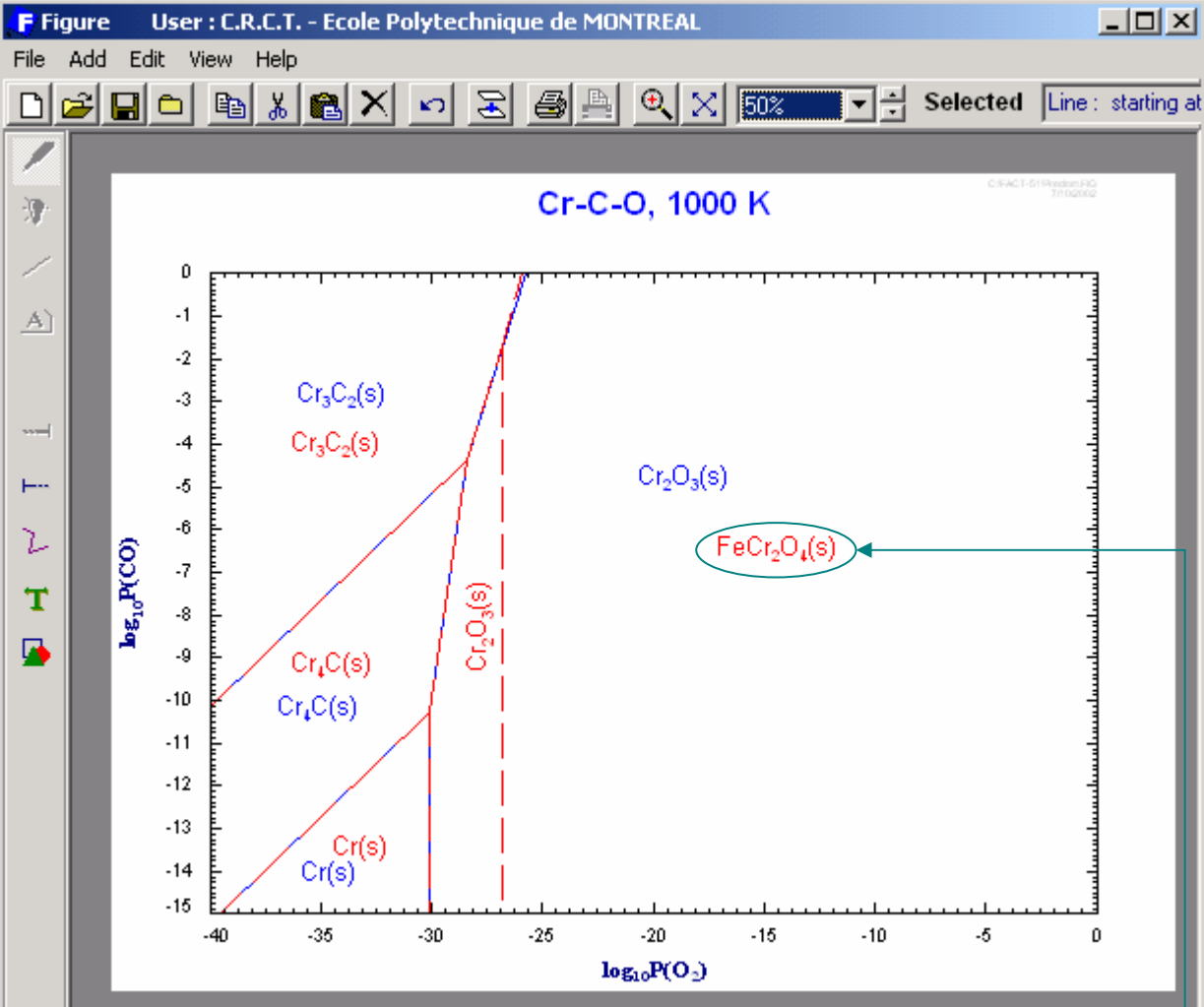
Parameters
Pressure: Isobar P(atm): 1.0
Constants: Temperature: 1000 Z: a[Fe(s)]
log10[Z]: 0

Calculate
diagram invariant point detailed point



Chromium-Carbon-Oxygen Predominance Diagram

Application: Decarburization of Chromium



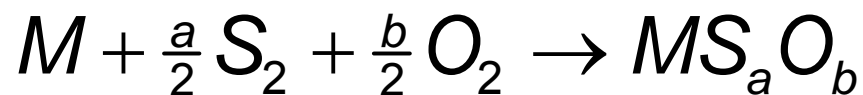
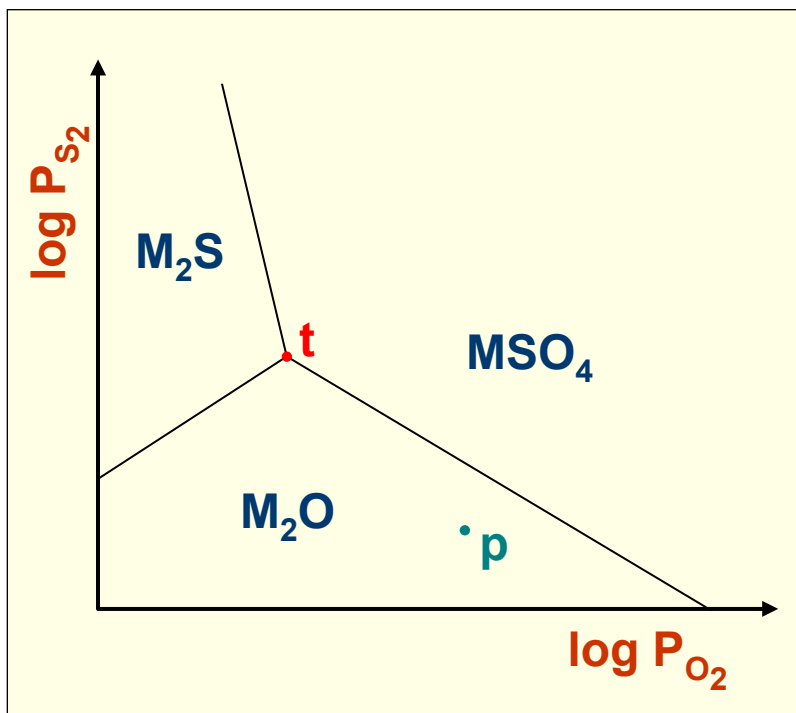
Use of the surimpose function of **Figure** (see Figure help, section 14) makes it easy to compare the **Cr-Fe-C-O** diagram (previous slide) with this **Cr-C-O** diagram to show the role of Fe in the formation of **FeCr₂O₄**

The following five slides give a detailed explanation on the stoichiometric relationships of the reactions that govern the phase boundaries in a predominance area diagram.

In principle there is no limitation in this approach as to the number of system components. However, there is one major restriction in the entire approach of using stoichiometric reactions: it is not suited for the treatment of systems with solution phases.

Basic computational procedure in the construction of a predominance diagram

Isothermal predominance diagram establishes at each $\log P_{S_2}$ and $\log P_{O_2}$ a particular compound MS_aO_b with the lowest ΔG of formation (based on 1 mole of M).



$$\Delta G_{MS_aO_b} = \Delta G_{MS_aO_b}^{\circ} + RT \ln \left(\frac{a_{MS_aO_b}}{a_M \cdot P_{S_2}^{\frac{a}{2}} \cdot P_{O_2}^{\frac{b}{2}}} \right)$$

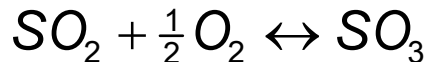
At point **p**, ΔG (for formation) of M_2O is most negative (per mole of M).
At point **t**, ΔG (for formation) of M_2O , M_2S and MSO_4 are equally negative.

Notes:

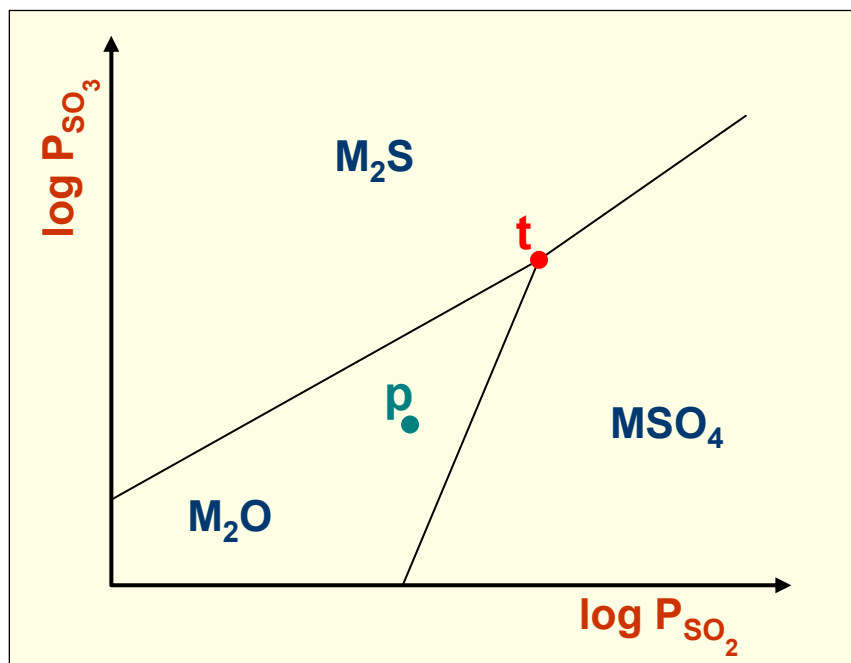
- It is not necessary to identify possible equilibria among phases by this method.
- The user may set $a_{MS_aO_b}$ or $P_{MS_aO_b}$ to other than 1 for some species.
Useful especially when MS_aO_b is a gaseous species.

Compounds as species represented on axes

Use of species other than elements for partial pressure associated with the axes. Select S-O species with different ratios of S/O for each axis. For example SO_2 and SO_3 :



At any coordinate, p , on the diagram, the partial pressure or chemical potential of elemental species O_2 or S_2 may be determined. The basic algorithm on the previous page can now be applied:

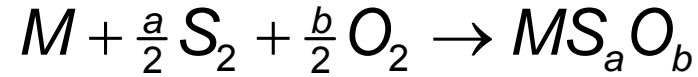
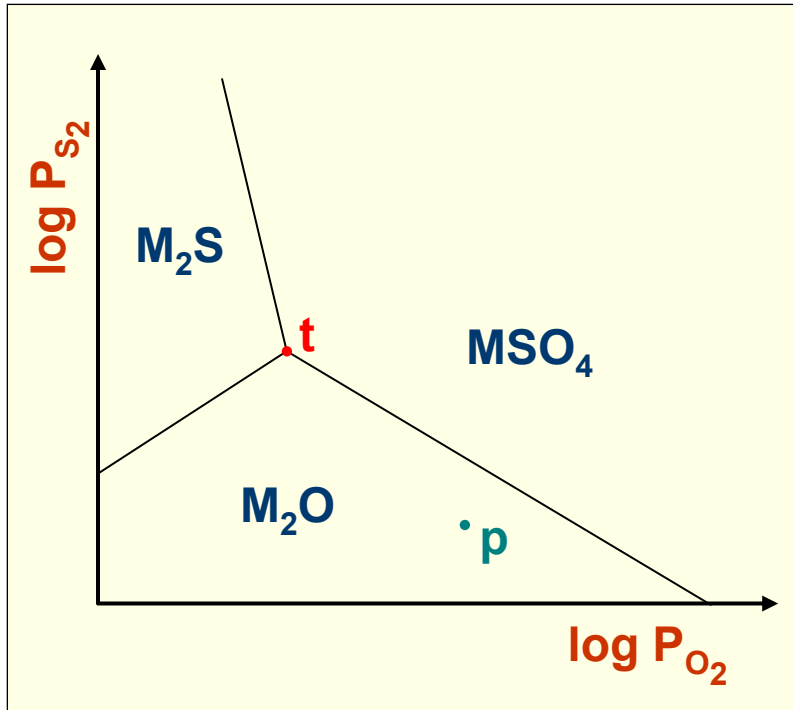


Notes:

- Species on axes must not contain the base element **M**
- Combination of species at triple point is independent of choice of S/O species for axes

Point calculation

At any particular point such as p in a known domain activity of M can be determined.



Insert a_M from above into equation below

$$\Delta G = RT \ln \left(\frac{a_{MS_aO_b}}{a_M \cdot P_{S_2}^{\frac{a}{2}} \cdot P_{O_2}^{\frac{b}{2}}} \right)$$

To find the activity of each MS_aO_b : $M + \frac{a}{2} S_2 + \frac{b}{2} O_2 \leftrightarrow MS_aO_b$

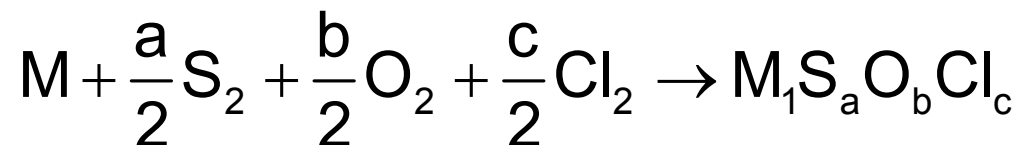
Activities and partial pressures of base-element-containing species at any point in the diagram. The activity of the particular species MS_aO_b identifying that domain is the set value (usually 1).

More than 3 Elements Involved in Diagram

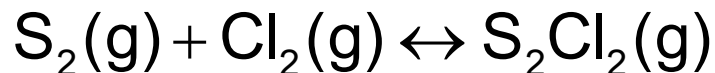
2 ways to proceed:

a) Fix additional chemical potentials (eg. P_{Cl_2})

Formulate formation reactions to construct the predominance area diagram shown in *Predom* 15 as follows:



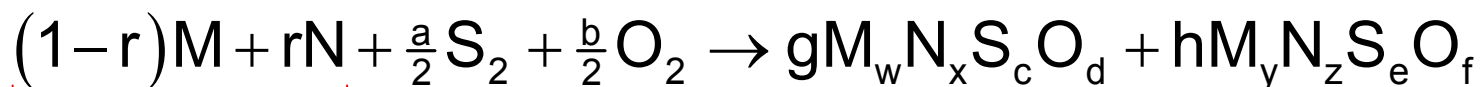
One can specify P_{Cl_2} for entire diagram, or as in *Predom* 15, specify partial pressure or activity of any Cl-S-O species (eg. S_2Cl_2)



By this equilibrium, one can find Cl_2 for any S_2 partial pressure

More than 3 Elements Involved in Diagram

b) Introduce an additional base element (eg. N)



Base elements
(specify range in
which r may be found)

Combination of two M and N containing
compounds which satisfy the mass
balances with non negative values for
g and h for a specified value of r

Note: In the case of a **two base element** diagram each domain is **doubly labelled**.
In the special case of there being no compounds containing both M and N,
the two base element diagram may be regarded simply as the
superimposition of the two one base element diagrams for M and N.