

# The *Phase Diagram* module

- Use the *Phase Diagram* module to generate various types of phase diagrams for systems containing stoichiometric phases as well as solution phases, and any number of system components.
- The *Phase Diagram* module accesses the compound and solution databases.
- The **graphical output** of the *Phase Diagram* module is handled by the *Figure* module.

## Table of contents

<b>Section 1</b>	<u>Table of contents</u>
<b>Section 2</b>	<u>Opening the Phase Diagram Module</u>
<b>Section 3</b>	<u>The various windows of the Phase diagram module</u>
<b>Section 4</b>	<u>Calculation of the phase diagram and graphical output</u>
<b>Section 5</b>	<u>Predominance area diagram (<b>Cu-SO<sub>2</sub>-O<sub>2</sub></b>)</u>
<b>Section 6</b>	<u>A metal-metal-oxygen diagram (<b>Fe-Cr-O<sub>2</sub></b>)</u>
<b>Section 7</b>	<u>A classical binary phase diagram (<b>Fe-Cr</b>)</u>

(continued)

## Table of contents (continued)

- Section 8**      A metal-oxygen diagram (**Fe-O<sub>2</sub>**)
- Section 9**      A ternary isopleth diagram (**Fe-C-W, 5 wt% W**)
- Section 10**     A quaternary predominance area diagram (**Fe-Cr-S<sub>2</sub>-O<sub>2</sub>**)
- Section 11**     A quaternary isopleth diagram (**Fe-Cr-V-C, 1.5% Cr, 0.1% V**)
- Section 12**     A ternary isothermal diagram (**CaO-Al<sub>2</sub>O<sub>3</sub>-SiO<sub>2</sub>**)
- Section 13**     Zero Phase Fraction (ZPF) Lines
- Section 14**     Generalized rules for the N-Component System
- Section 15**     Using the rules for classical cases
  - MgO-CaO** Binary System
  - Fe - Cr - S<sub>2</sub> - O<sub>2</sub>** System
- Section 16**     Breaking the rules: Diagrams - but not phase diagrams
  - Pressure vs. Volume diagram for H<sub>2</sub>O
  - Composition and activity of a component (**Fe - Cr - C**)

# Initiating the *Phase Diagram* module



Click on *Phase Diagram* in the main *FactSage* window.

Calculate and plot phase diagrams

# The various windows and screens of **Phase Diagram**

The following three slides show how a phase diagram calculation is prepared via

the **Components input** window,

then the **Phase Diagram menu window**, and finally

the **Variables window**.

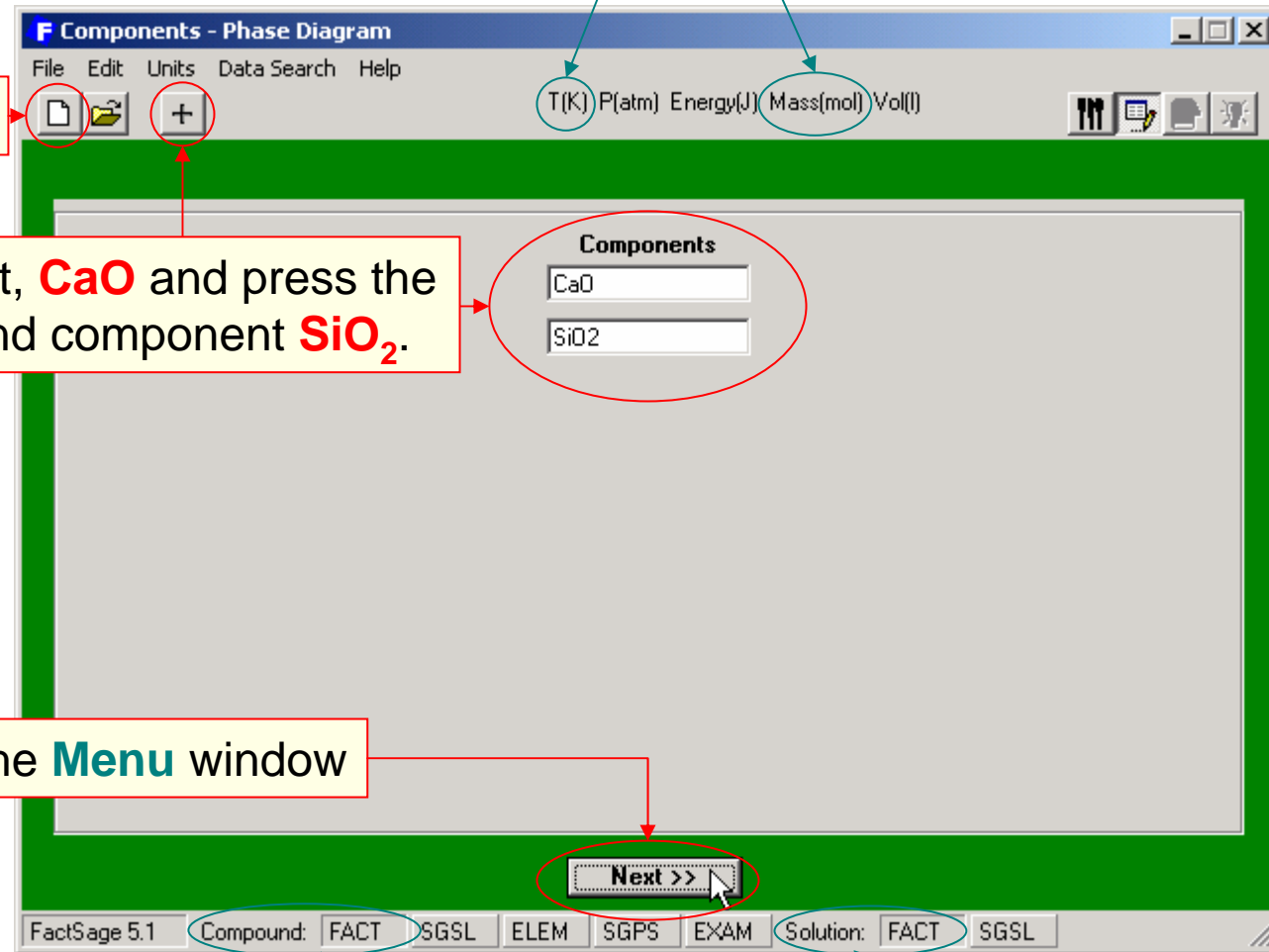
# Components window – preparing a new *Phase Diagram*: CaO – SiO<sub>2</sub>

Calculation of the CaO-SiO<sub>2</sub> binary phase diagram – T(K) vs. X(SiO<sub>2</sub>)

1° Click on the **New** button

2° Enter the first component, **CaO** and press the **+** button to add the second component **SiO<sub>2</sub>**.

3° Press **Next >>** to go to the **Menu** window



The **FACT** Compound and solution databases are used.

# Menu window – selection of the compound and solution species

1° **Select** the products to be included in the calculation:  
pure solid compound species and the liquid slag phase.

**F Menu - Phase Diagram**  
File Units Parameters **Variables** Help

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

**Components (2)**  
CaO + SiO2

**Products**  
Compound species  
 gas  ideal  real 0  
 liquid 0  
 aqueous 0  
 solid 23  
 suppress duplicates  
Species: 23

**Solution species**

*	+	Base-Phase	Full Name
		FACT-SLAG	Slag-liquid

**Variables**

T(K)	SiO2/(CaO+SiO2)			
300 1500	0 1			

T(K) vs SiO2/(CaO+SiO2)

FactSage 5.1

2° **Right-click** to display the extended menu on **FACT-SLAG**.

Solution **FACT-SLAG**

- clear
- ✓ - all species
- \* - custom select species ...
- ✓ + - single phase
- I - possible 2-phase immiscibility**
- ! - possible 3-phase immiscibility
- ✓ - standard stable phase
- ! - dormant (metastable) phase
- Help ...

3° Select the option possible **2-phase immiscibility**

**Solution species**

*	+	Base-Phase	Full Name
		FACT-SLAG	Slag-liquid

**Legend**  
I - immiscible

species: 4  
solutions: 2

4° **Click** in the **Variables' boxes** to open the Variables window (clicking on **Variables** in the menu bar does the same).

# Variables window – defining the variables for the phase diagram

Calculation of the CaO-SiO<sub>2</sub> binary phase diagram – **T(K)** vs. **X(SiO<sub>2</sub>)**

1° **Select** a X-Y (rectangular) graph and **one** composition variable: **X(SiO<sub>2</sub>)**

2° **Press Next >>** to define the composition, temperature and pressure.

3° **Set the Temperature** as Y-axis and **enter** its limits.

The screenshot shows a software window titled "Variables: CaO-SiO2 T(K) vs composition #1." with several sections:

- Variables:** A graph icon with 'Y' and 'X' axes. Below it, a triangle with vertices 'A', 'B', and 'C'. 'Y steps' and 'X steps' are both set to 5. A "Next >>" button is highlighted with a red box.
- T and P:** Two sub-sections. The "Temperature" section has radio buttons for "T(K)" (selected) and "1/TK". "T(K)" is set to "Y-axis" with a "Max:" of 3000 and "Min:" of 1000. The "Pressure" section has radio buttons for "P(atm)" (selected) and "log P". "P(atm)" is set to "constant" with a value of 1. A red box highlights the "P(atm)" section.
- Compositions (mole):** A section with two rows. The first row is "0 CaO + 1 SiO2" with a dropdown set to "X-axis". The second row is "1 CaO + 1 SiO2". To the right, there are input fields for "1 (max)" and "0 (min)". A red box highlights this section.
- At the bottom, there are "Cancel" and "OK" buttons. The "OK" button is circled in red.

4° **Set the Pressure** at 1 atm.

5° **Set the composition** [mole fraction **X(SiO<sub>2</sub>)**] as X-axis and **enter** its limits.

6° **Press OK** to return to the **Menu** window.

# Calculation of a Phase Diagram and Graphical Output

In the following two slides a **summary of the input** concerning the axes of a phase diagram is given (**axes variable and their ranges**) and it is shown how the phase diagram once calculated is «**post-processed**» in the **Figure** module in terms of **adding labels** into the various phase fields of the diagram.



# Phase Diagram and Variables frames

## Phase Diagram Frame

Press **Calculate**>> to generate the phase diagram using the **Figure** module.

Variables				
T(K)	SiO <sub>2</sub> /(CaO+SiO <sub>2</sub> )			
1000 3000	0 1			

T(K) vs SiO<sub>2</sub>/(CaO+SiO<sub>2</sub>)

Phase Diagram

Y  
X

Calculate >>

## Variables Frame

Click in the **Variables'** boxes to open the **Variables window**

The variables window changes appearance according to your choice of variables.

See the following chapters for further examples.

**F Variables: CaO-SiO<sub>2</sub> T(K) vs composition #1.**

**Variables**

Y  
 X

composition   
log<sub>10</sub>(a)   
RTln(a)

Y steps:   
X steps:

Next >>

**T and P**

Temperature

T(K)  1/TK  
Y-axis  
Max:   
Min:

Pressure

P(atm)  log P  
constant

**Compositions (mole)**

#1.  CaO +  SiO<sub>2</sub> =   
 CaO +  SiO<sub>2</sub> =

Cancel OK

# Calculation of the phase diagram and graphical output

1° Press Calculate>> to view the resulting phase diagram.

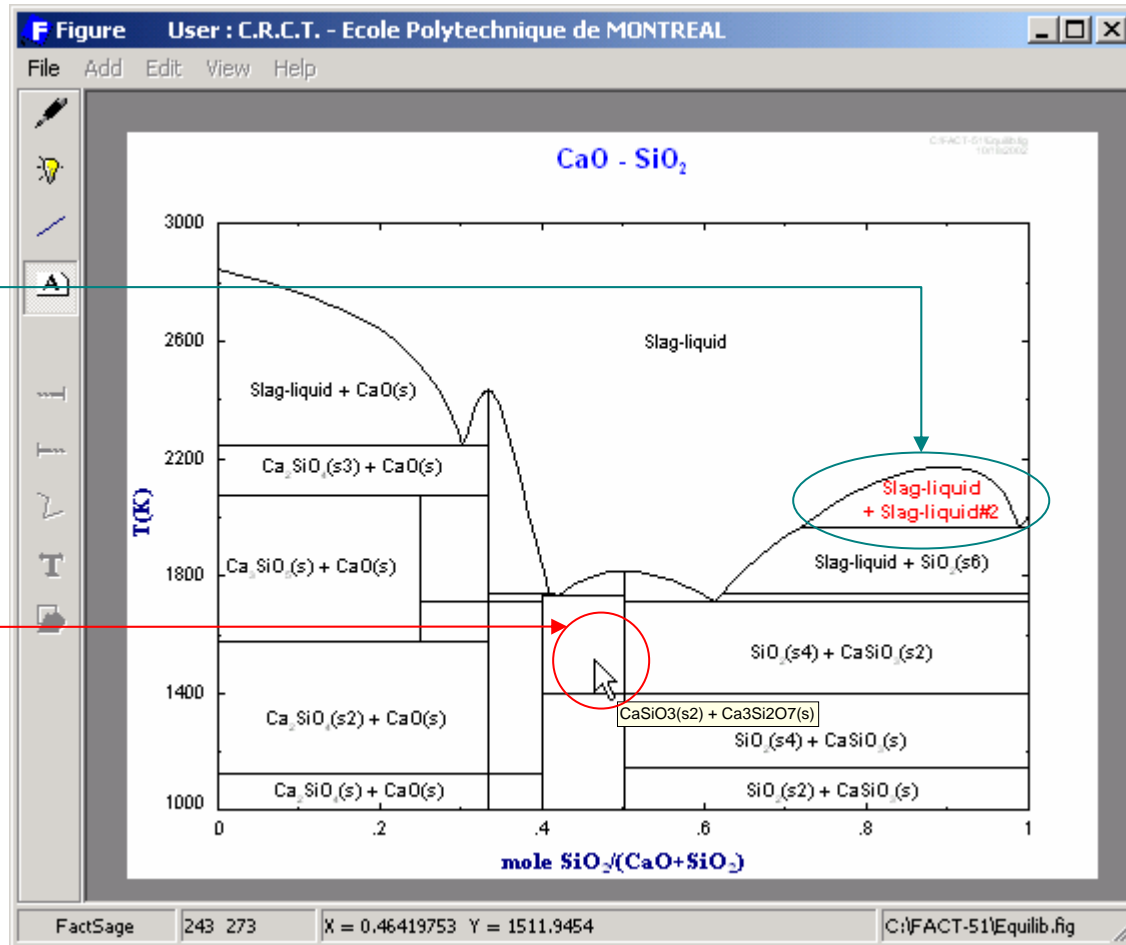
Variables	
T(K)	SiO <sub>2</sub> /(CaO+SiO <sub>2</sub> )
1000 3000	0 1

T(K) vs SiO<sub>2</sub>/(CaO+SiO<sub>2</sub>)

Phase Diagram

Calculate >>

Note the effect of the **I** option: the miscibility gap is calculated.



2° You can point and click to label the phase diagram.

See the **Figure** slide show for more features of the **Figure** module.

# A classical predominance area diagram

In the following two slides is shown how the *Phase Diagram* module is employed in order to generate the same type of diagram that can also be produced with the *Predom* module.

As an example the system is **Cu-SO<sub>2</sub>-O<sub>2</sub>**.

Note that SO<sub>2</sub> and O<sub>2</sub> are used as input in the *Components window*.

# Predominance area diagram: $\text{Cu-SO}_2\text{-O}_2$ ; Data Input

1° **Entry** of the components  
(done in the **Components** window)

2° **Definition** of the variables:

- **Chemical potentials**
- **T = 1000K**
- **P = 1 atm**

**Components (3)**  
SO2 + O2 + Cu

**Products**

Compound species:

- gas ideal real 19
- liquid 0
- aqueous 0
- solid 13

suppress duplicates  
Species: 32

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

**Solution species**

	+	Base-Phase	Full Name
		FACT-SLAG	Slag-liquid
		FACT-CuLQ	Cu-liq
		FACT-MATT	Matte

Legend:  Show  all  selected  
species: 0  
solutions: 0

**Variables**

T(K)	log10(p(SO2))	log10(p(O2))	
1000	-12.8	-20.0	

log10(p(SO2)) vs log10(p(O2))

Calculate >>>

3° **Selection** of the products:

- **Gas ideal**
- **Solid**

4° **Computation** of the phase diagram

**Variables: SO2-O2-Cu log10(p(SO2)) vs log10(p(O2))**

**Variables**

composition 0  
log10(a) 2  
RTln(a) 0

**T and P**

Temperature:  T(K) constant 1000  
 1/TK 1000

Pressure:  P(atm) constant 1  
 log P 1

**Chemical Potentials**

#1. log10(p) = Y-axis

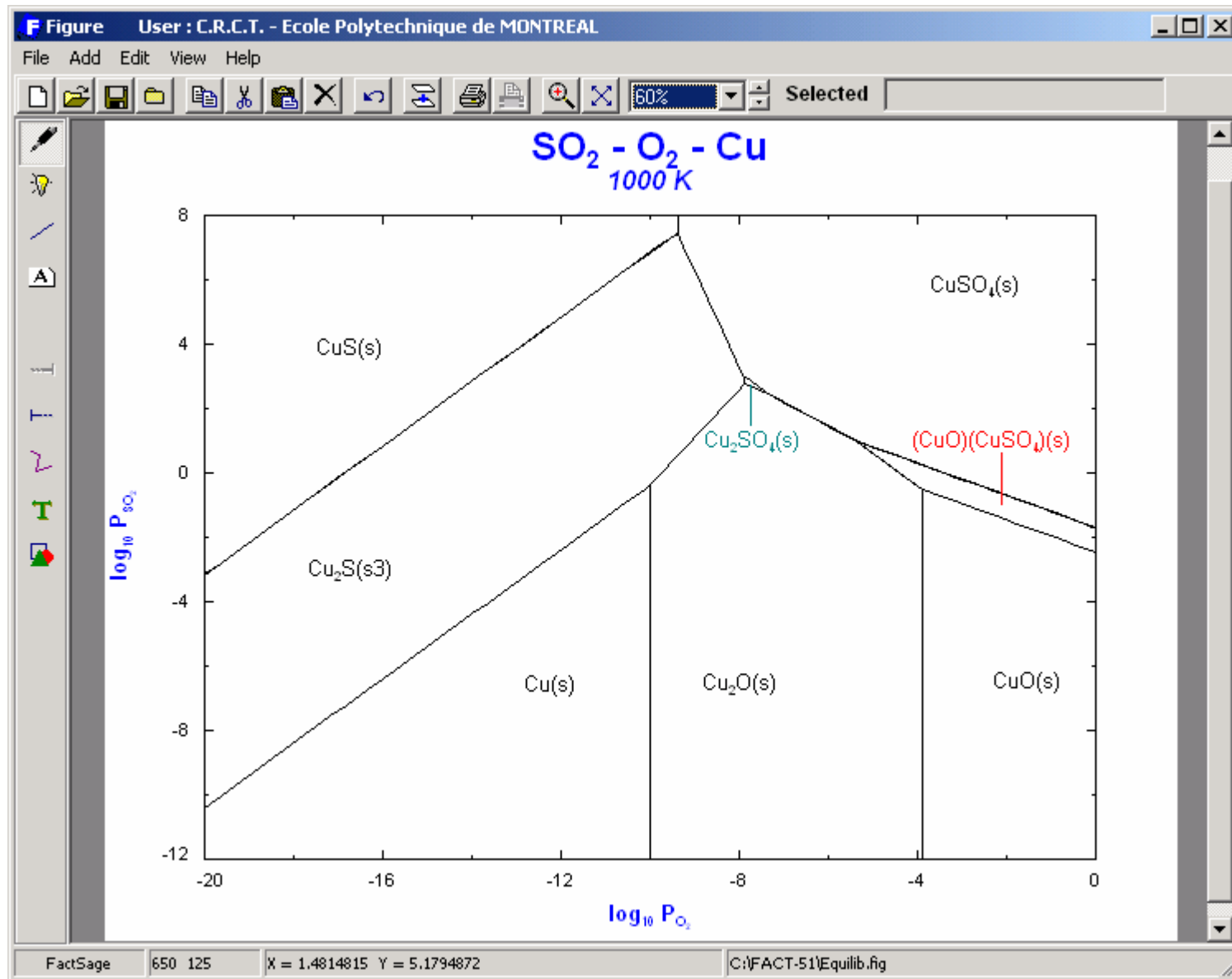
SO2	8
gas	-12

#2. log10(p) = X-axis

O2	0
gas	-20

Cancel OK

# Predominance area diagram: $\text{Cu-SO}_2\text{-O}_2$ ; Graphical Output



# A two metal oxygen system

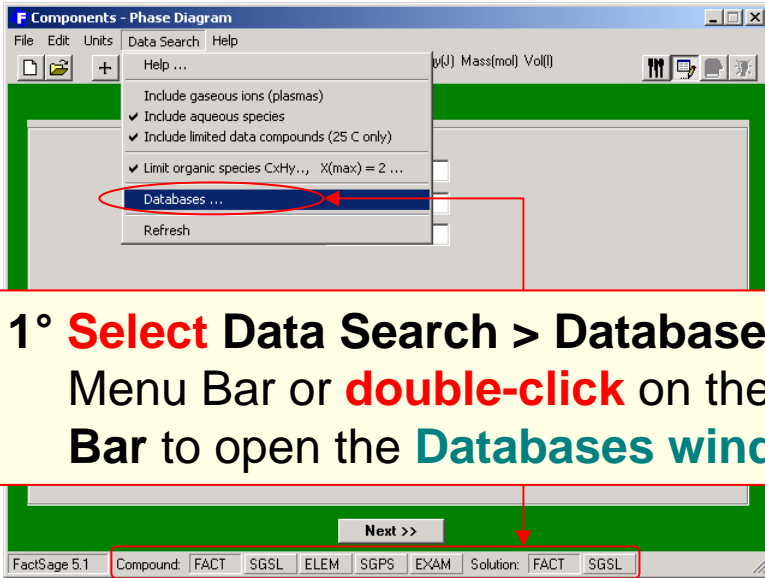
In the following three slides is shown how a phase diagram for an alloy system with **variable composition** under a gas phase with **variable oxygen potential** (partial pressure) for constant temperature is prepared and generated.

As an example the system is **Fe-Cr-O<sub>2</sub>**.

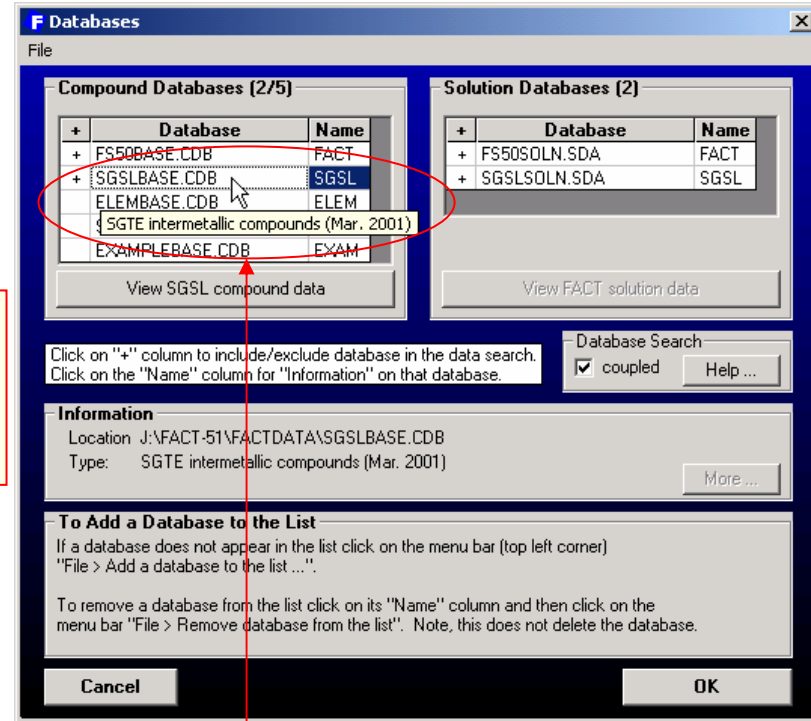
Note the use of the «**metallic mole fraction**» ( $\text{Cr}/(\text{Cr}+\text{Fe})$ ) on the x-axis while the oxygen partial pressure is used as  $\log P(\text{O}_2)$  on the y-axis.

Also note the combined use of the FACT (for the oxides) and the SGTE (SGSL, for the alloy solid solutions) databases.

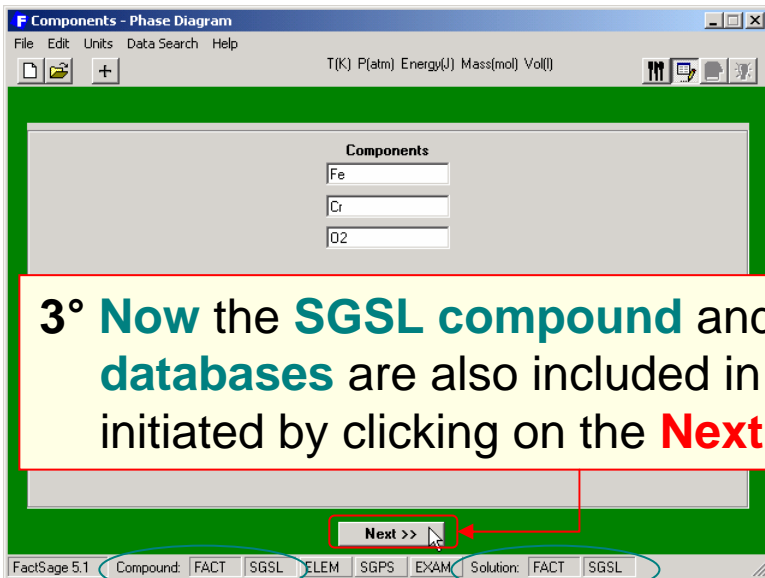
# Fe-Cr-O<sub>2</sub>: addition of a database



1° **Select Data Search > Databases...** from the Menu Bar or **double-click** on the **Databases Bar** to open the **Databases window**.



2° **Click** on '+' column to **include** or **exclude** a **database** from the data search.



3° **Now the SGSL compound and solution databases** are also included in the data search initiated by clicking on the **Next** button.

# Fe-Cr-O<sub>2</sub>: selection of variables and solution phases

1° **Entry** of the components  
(done in the **Components** window)

2° **Definition** of the variables:

- 1 **Chemical Potential**:  $P(\text{O}_2)$
- 1 **Composition**:  $X_{\text{Cr}}$
- $T = 1573\text{K}$
- $P = 1\text{ atm}$

**F Menu - Phase Diagram**

File Units Parameters Variables Help

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

Components (3)

Fe + Cr + O<sub>2</sub>

Products

Compound species:

- gas  ideal  real 9
- liquid 0
- aqueous 0
- solid 21
- suppress duplicates

Species: 30

Target: - none -

Estimate T(K): 1000

Mass(mol): 0

Solution species

	+	Base-Phase	Full Name
<input checked="" type="checkbox"/>		FACT-FeSP	FeSpinel
<input checked="" type="checkbox"/>		FACT-MeO	Monoxide
<input checked="" type="checkbox"/>		FACT-CORU	M2O3(Corundum)
<input checked="" type="checkbox"/>		SGSL-FCC	FCC_A1
<input checked="" type="checkbox"/>		SGSL-BCC	BCC_A2

Legend: +- selected

Show  all  selected

species: 12

solutions: 5

Clear

Variables

T(K)	log10(p(O <sub>2</sub> ))	Cr/(Fe+Cr)
1573	-20.0	0.1

log10(p(O<sub>2</sub>)) vs Cr/(Fe+Cr)

Phase Diagram

Calculate >>

3° **Selection** of the products:

- **Gas ideal**
- **Solid**
- **And 5 solution phases**

4° **Computation** of the phase diagram

**F Variables: Fe-Cr-O<sub>2</sub> log10(p(O<sub>2</sub>)) vs composition #1.**

Variables

composition 1

log10(a) 1

RTln(a) 0

Y steps: 5

X steps: 5

Next >>

T and P

Temperature

T(K) constant 1573

1/TK

Pressure

P(atm) constant 1

log P

Chemical Potentials

#1. log10(p) = Y-axis

O<sub>2</sub> 0 (max)

gas-FACT -20 (min)

Compositions (mole)

#1. 0 Fe + 1 Cr = X-axis

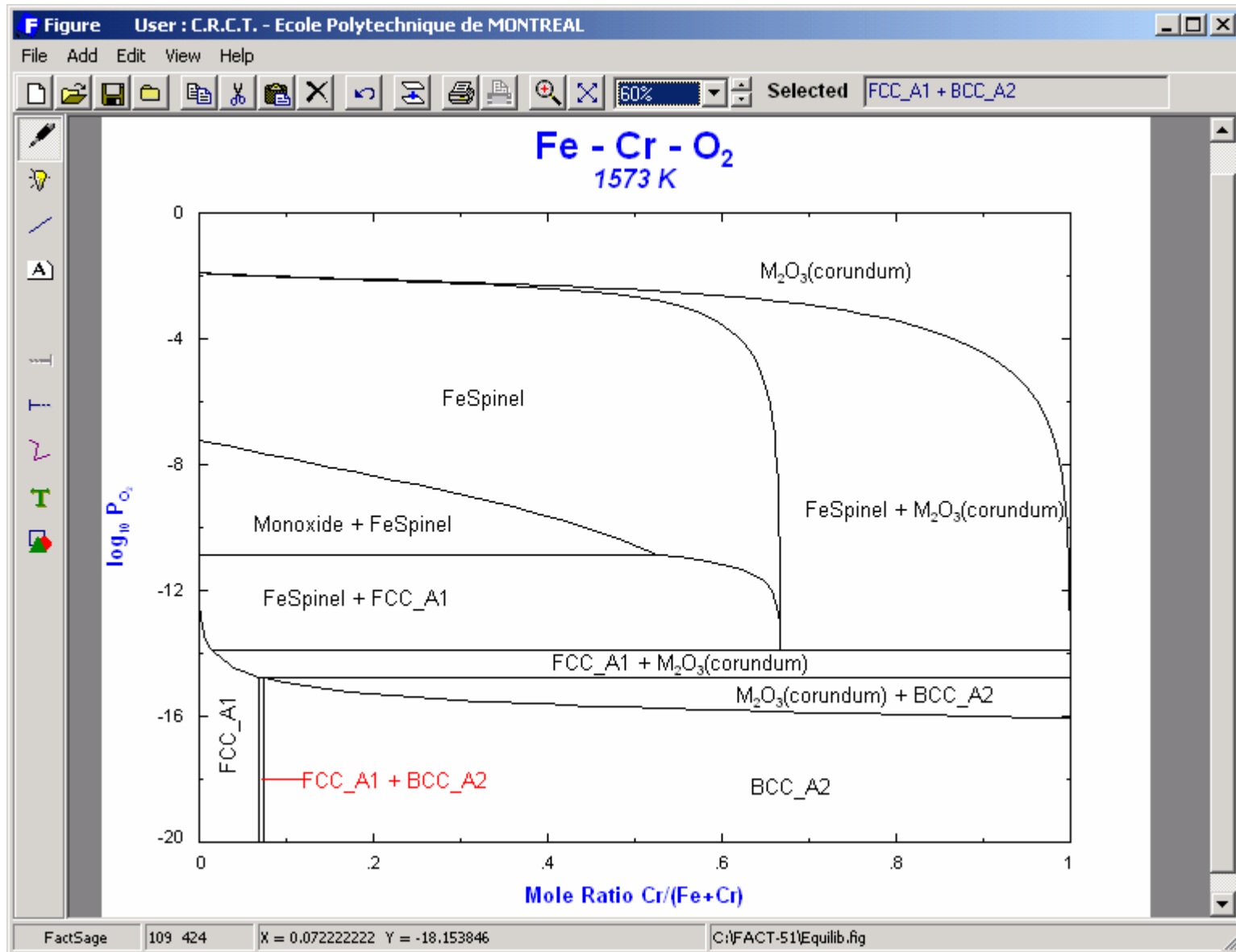
1 Fe + 1 Cr = 1 (max)

0 (min)

Cancel OK



# Fe-Cr-O<sub>2</sub> : graphical output



# A classical temperature vs composition diagram

The following two slides show the preparation and generation of a labelled **binary T vs X phase diagram**.

Note: The labels are entered into the diagram interactively. Click on the «A» button (stable phases label mode) and then move the cursor through the diagram. Where the left mouse button is clicked a label will be inserted into the diagram.

The **Fe-Cr system** is used in this example.

# Fe-Cr binary phase diagram: input variables and solution species

1° **Entry** of the components  
(done in the **Components** window)

- 2° **Definition** of the variables:
- **Composition:**  $0 < Wt_{Cr} < 1$
  - $500K < T < 2300K$
  - $P = 1 \text{ atm}$

**Components** [2] (gram) Fe + Cr

**Products**

Compound species	gas	ideal	real	0
liquid	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	0
aqueous	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	0
solid	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	0
suppress duplicates	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>

Species: 0

**Solution species**

	+	Base-Phase	Full Name
<input type="checkbox"/>	<input checked="" type="checkbox"/>	SGSL-FCC	FCC_A1
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	SGSL-BCC	BCC_A2
<input type="checkbox"/>	<input checked="" type="checkbox"/>	SGSL-SIGM	SIGMA
<input type="checkbox"/>	<input checked="" type="checkbox"/>	SGSL-LIQU	LIQUID

Legend: - immiscible, + selected

show:  all,  selected

species: 10, solutions: 5

**Variables**

T(K)	Cr/(Fe+Cr)			
500	2300	0.1		

T(K) vs Cr/(Fe+Cr)

**Phase Diagram**

Calculate >>

3° **Selection** of the products:

- 3 solid solution phases
- 1 liquid solution phase

Note the immiscibility for the BCC phase

4° **Computation** of the phase diagram

**Variables**

composition 1

log10(a) 0

RTln(a) 0

Y steps: 5

X steps: 5

Next >>

**T and P**

Temperature: T(K) Y-axis, 1/TK Max: 2300, Min: 500

Pressure: P(atm) constant, log P 1

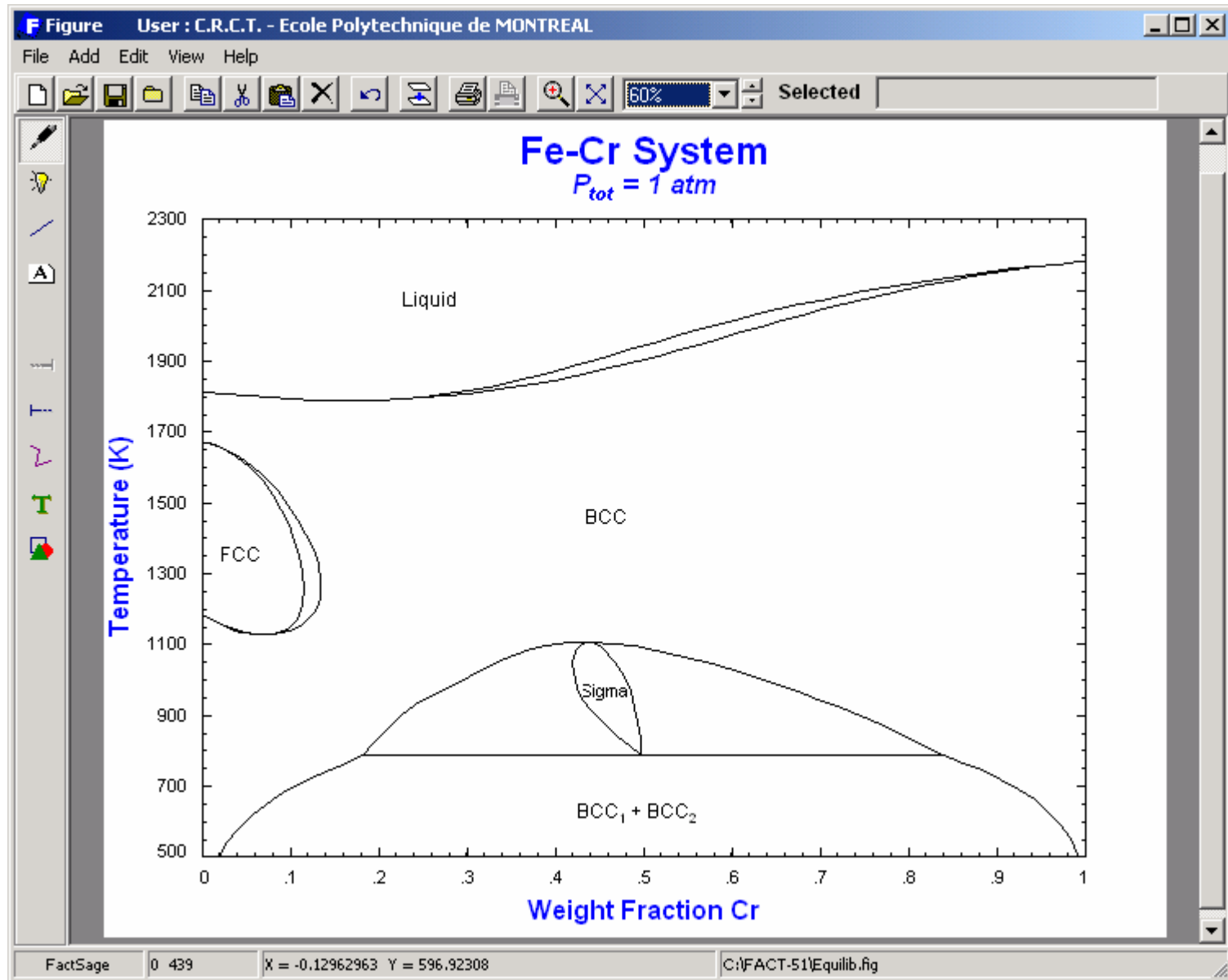
**Compositions (mass)**

#1. 0 Fe + 1 Cr = 1 (max) X-axis

1 Fe + 1 Cr = 0 (min)

Cancel OK

# Fe-Cr binary phase diagram: graphical output



# A **two potential** phase diagram

In the following two slides the preparation and generation of a phase diagram with **two potential axes** is shown.

The chosen axes are temperature and one **chemical potential** in a **binary system**. Note the **difference in the diagram topology** that results from the choice of  $RT \ln P(\text{O}_2)$  rather than  $\log P(\text{O}_2)$ .

The **Fe-O<sub>2</sub>** system is used as the example.

# Fe-O<sub>2</sub> system: input

1° **Entry** of the components  
(done in the **Components** window)

2° **Definition** of the variables:

- **1 Chemical potential**
- **700K < T < 2000K**
- **P = 1 atm**

**Components** [2]

Fe + O<sub>2</sub>

**Products**

Compound species:

- gas  ideal  real 0
- liquid  0
- aqueous  0
- solid  10

suppress duplicates

Species: 10

Target: - none -

Estimate T(K): 1000

Mass(mol): 0

**Solution species**

+	Base-Phase	Full Name
+	FACT-SLAG	Slag-liquid
+	FACT-SPIN	Spinel
+	FACT-MeO	Monoxide
+	FACT-FeLQ	Fe-liq
+	FACT-CuLQ	Cu-liq

Legend: + - selected

Show  all  selected

species: 12

solutions: 4

Clear

**Variables**

T(K)	RTln(p(O <sub>2</sub> ))			
700	2000	-500000	100000	

T(K) vs RTln(p(O<sub>2</sub>))

Calculate >>

3° **Selection** of the products:

- **Solid**
- **4 solution phases**

4° **Computation** of the phase diagram

**Variables**

composition 0

log10(a) 0

RTln(a) 1

Y steps: 5

X steps: 5

Next >>

**T and P**

Temperature: T(K) Y-axis

Max: 2000

Min: 700

Pressure: P(atm) constant

log P 1

**Chemical Potentials**

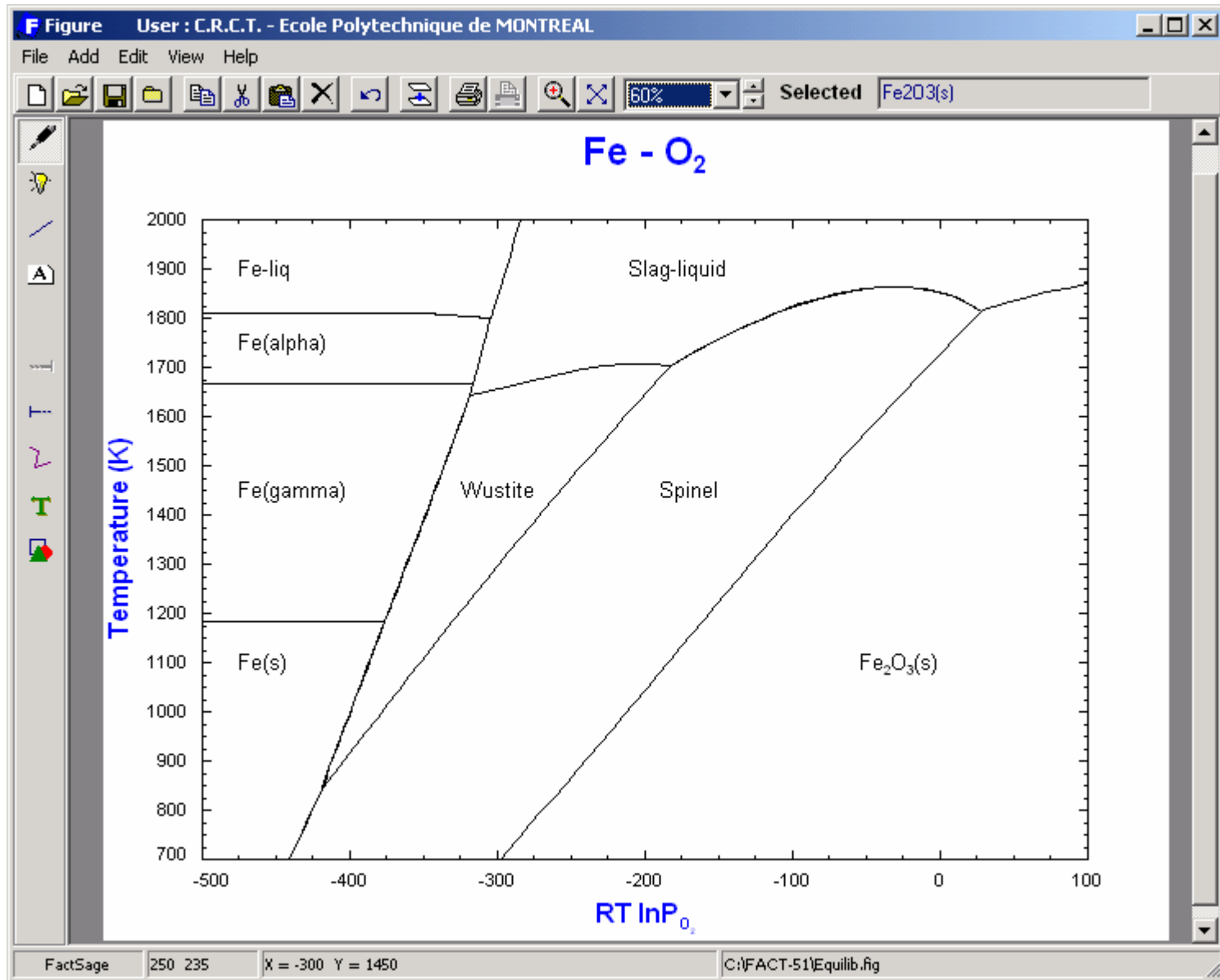
#1. RTln(p) = X-axis

O<sub>2</sub> 100000

gas -500000

Cancel OK

# Fe-O<sub>2</sub> system: graphical output



# A ternary isopleth diagram

The following two slides show how a **ternary isopleth diagram** is prepared and generated.

Temperature and one weight percent variable are used on the axes while the **third compositional variable** (here the wt% of the second metallic component) is kept constant.

As an example the **Fe-W-C system** is used.



# Fe-C-W system at 5 wt% W: **input**

1° **Entry** of the components  
(done in the **Components** window)

2° **Definition** of the variables:

- **2 compositions (mass)**
- **900K < T < 1900K**
- **P = 1 atm**

**F Menu - Phase Diagram**

File Units Parameters Variables Help

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

Components (3)  
(gram) Fe + C + W

Products

Compound species

gas  ideal  real 0  
liquid  0  
aqueous  0  
 solid 13  
 suppress duplicates

Species: 13

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

Solution species

+	Base-Phase	Full Name
+	SGSL-FCC	FCC_A1
+	SGSL-BCC	BCC_A2
+	SGSL-CEME	CEMENTITE
+	SGSL-LIQU	LIQUID
+	SGSL-M6C	M6C
+	SGSL-M7C3	M7C3
+	SGSL-M236	M23C6

Legend  
+ - selected  Show  all  selected  
species: 19  
solutions: 7

Variables

T(K)	C/(Fe+C+W)	W/(Fe+C+W)
900 1900	0 0.02	0.05

Phase Diagram  
Y  
X  
**Calculate >>**

3° **Selection** of the products:

- **Solid** (compound species)
- **7 solution phases**

4° **Computation** of the phase diagram

**F Variables: Fe-C-W T(K) vs composition #1.**

Variables

Y  composition 2  
X  log10(a) 0  
 RTln(a) 0  
Y steps: 5  
X steps: 5  
Next >>

T and P

Temperature  
 T(K) Y-axis  
Max: 1900  
Min: 900  
 1/TK

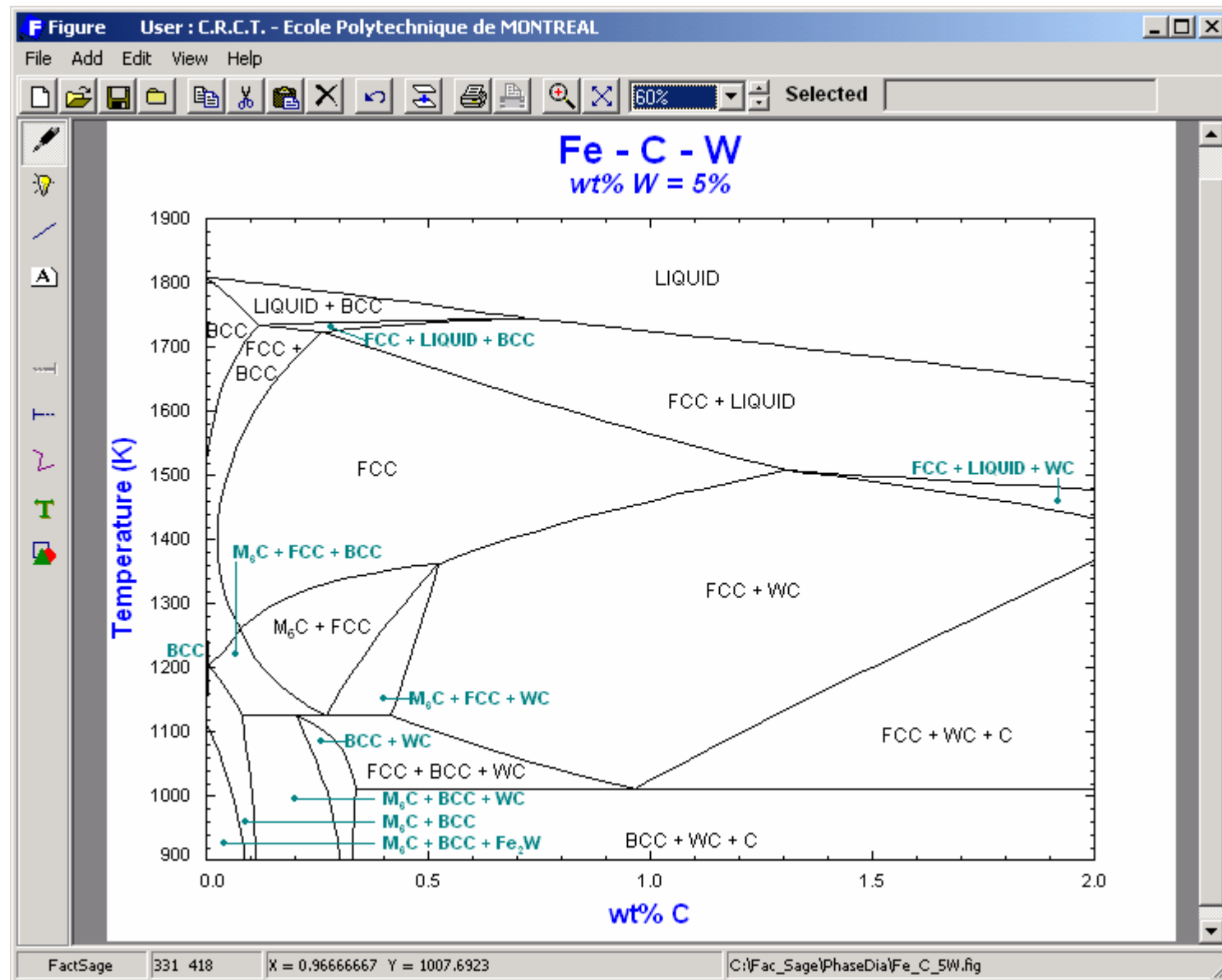
Pressure  
 P(atm) constant  
 log P 1

Compositions [mass]

#	Fe	C	W	Y-axis
#1.	0	1	0	0.02 (max)
	1	1	1	0 (min)
#2.	0	0	1	constant
	1	1	1	0.05

Cancel OK

# Fe-C-W system at 5 wt% W: graphical output



# A quaternary predominance area diagram

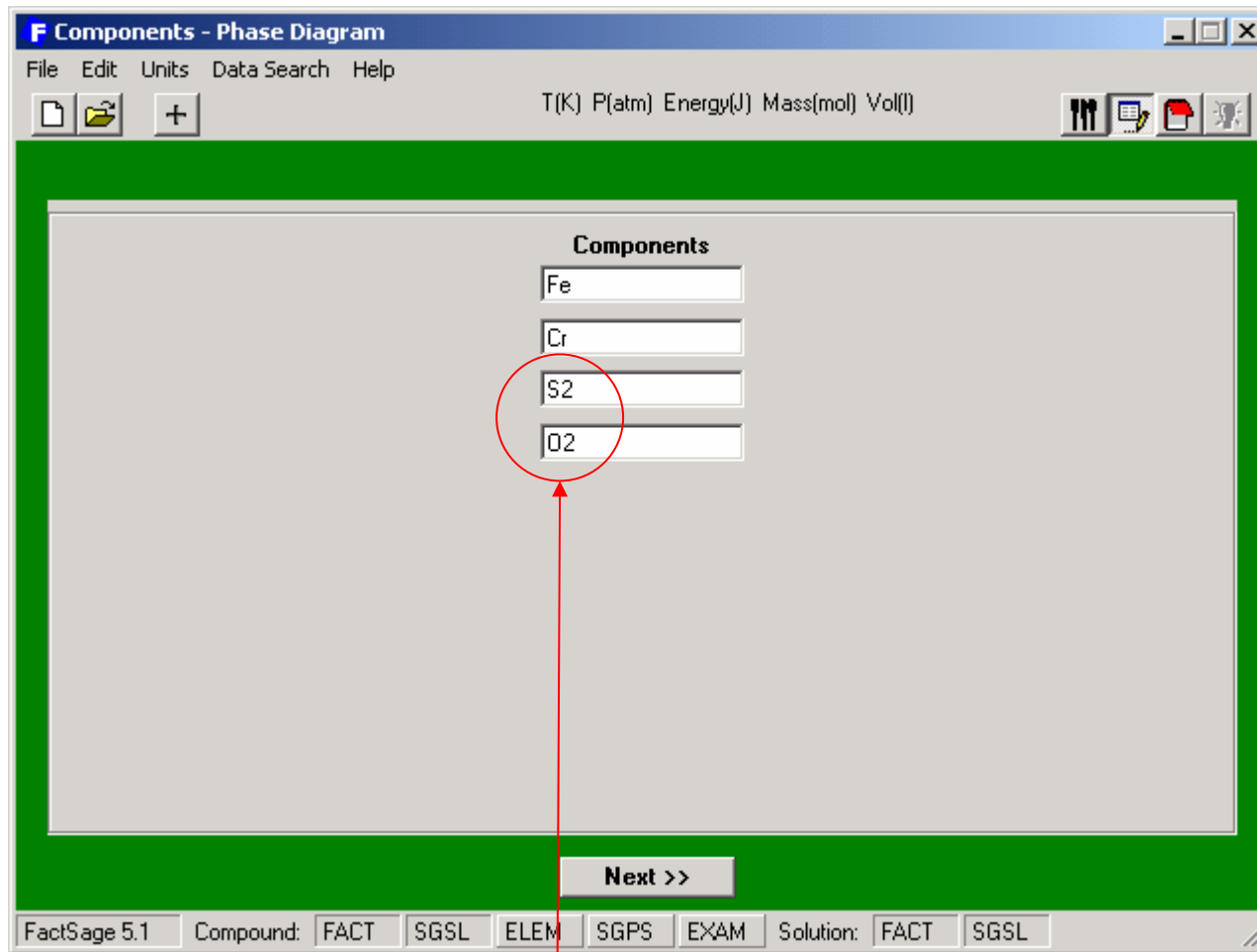
The following three slides show the **preparation and calculation** of a **predominance area type phase diagram** with **two metal components** and **two gaseous components**.

The partial pressures, i.e. chemical potentials, of the gaseous components are used as axes variables. Note the use of the species names  $O_2$  and  $S_2$  in the Components window. These are used to retrieve the data for the correct gas species from the database. Temperature and total pressure are kept constant.

Different from the Predom module the present diagram also shows **the effect of solution phase formation** (FCC, BCC, (Fe,Cr)S, Fe-spinel).

As an example the **Fe-Cr-S<sub>2</sub>-O<sub>2</sub>** system is used.

# Predominance area diagram: Fe-Cr-S<sub>2</sub>-O<sub>2</sub> System, solid solution **input**



**Note** the chemical formula of the gas components.  
These are used because  $\log p_{\text{O}_2}$  and  $\log p_{\text{S}_2}$  are going to be axes variables.

# Fe-Cr-S<sub>2</sub>-O<sub>2</sub> System, variable and solid solution **input**

1° **Entry** of the components  
(done in the **Components** window)

- 2° **Definition** of the variables:
- 1 **Composition**:  $X_{Cr} = 0.5$
  - 2 **Chemical Potentials**:  $P(O_2)$  and  $P(S_2)$  (on axes)
  - $T = 1273K$
  - $P = 1 \text{ atm}$

**Menu - Phase Diagram**

File Units Parameters Variables Help

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

**Components (4)**

Fe + Cr + S<sub>2</sub> + O<sub>2</sub>

**Products**

Compound species

gas  ideal  real 0

liquid  0

aqueous  0

solid  2

suppress duplicates

\* - custom selection

Species: 2

Target: - none -

Estimate T(K): 1000

Mass(mol): 0

**Solution species**

*	+	Base-Phase	Full Name
		FACT-FeSP	FeSpinel
		FACT-MeO	Monoxide
		FACT-CORU	M2O3(Corundum)
		SGSL-FCC	FCC_A1
		SGSL-BCC	BCC_A2
		SGSL-SIGM	SIGMA

Legend

! - immiscible

+ - selected

species: 20

solutions: 7

Clear

**Variables**

T(K)	log10(p(S <sub>2</sub> ))	log10(p(O <sub>2</sub> ))	Cr/(Fe+Cr)
1273	-10.0	-25.10	0.5

log10(p(S<sub>2</sub>)) vs log10(p(O<sub>2</sub>))

FactSage 5

**Custom Solutions**

Fixed Activity: 0 Species

Ideal Solution:

#1 (Fe,Cr)S<sub>2</sub>-

53: CrS(s)

72: FeS(s)

OK

Custom Solutions:

0 fixed activities

1 ideal solutions

0 activity coefficients

Details ...

Pseudonyms:

apply  List ...

include molar volumes

Total Species [max 692] 22

Total Solutions [max 30] 8

Default

**Phase Diagram**

Y

X

Calculate >>

- 3° **Selection** of the products:
- **Solid (custom selection: an ideal solution)**
  - **6 solution phases** (including one with a possible miscibility gap)

4° **Computation** of the phase diagram

**Variables: Fe-Cr-S2-O2 log10(p(S<sub>2</sub>)) vs log10(p(O<sub>2</sub>))**

Variables

composition 1

log10(a) 2

RTln(a) 0

Y steps: 5

X steps: 5

Next >>

**T and P**

Temperature

Pressure

T(K) constant

P(atm) constant

1/TK 1273

log P 1

**Chemical Potentials**

#1. log10(p) = Y-axis

S<sub>2</sub> 0

gas-FACT -10

#2. log10(p) = X-axis

O<sub>2</sub> -10

gas-FACT -25

**Compositions (mole)**

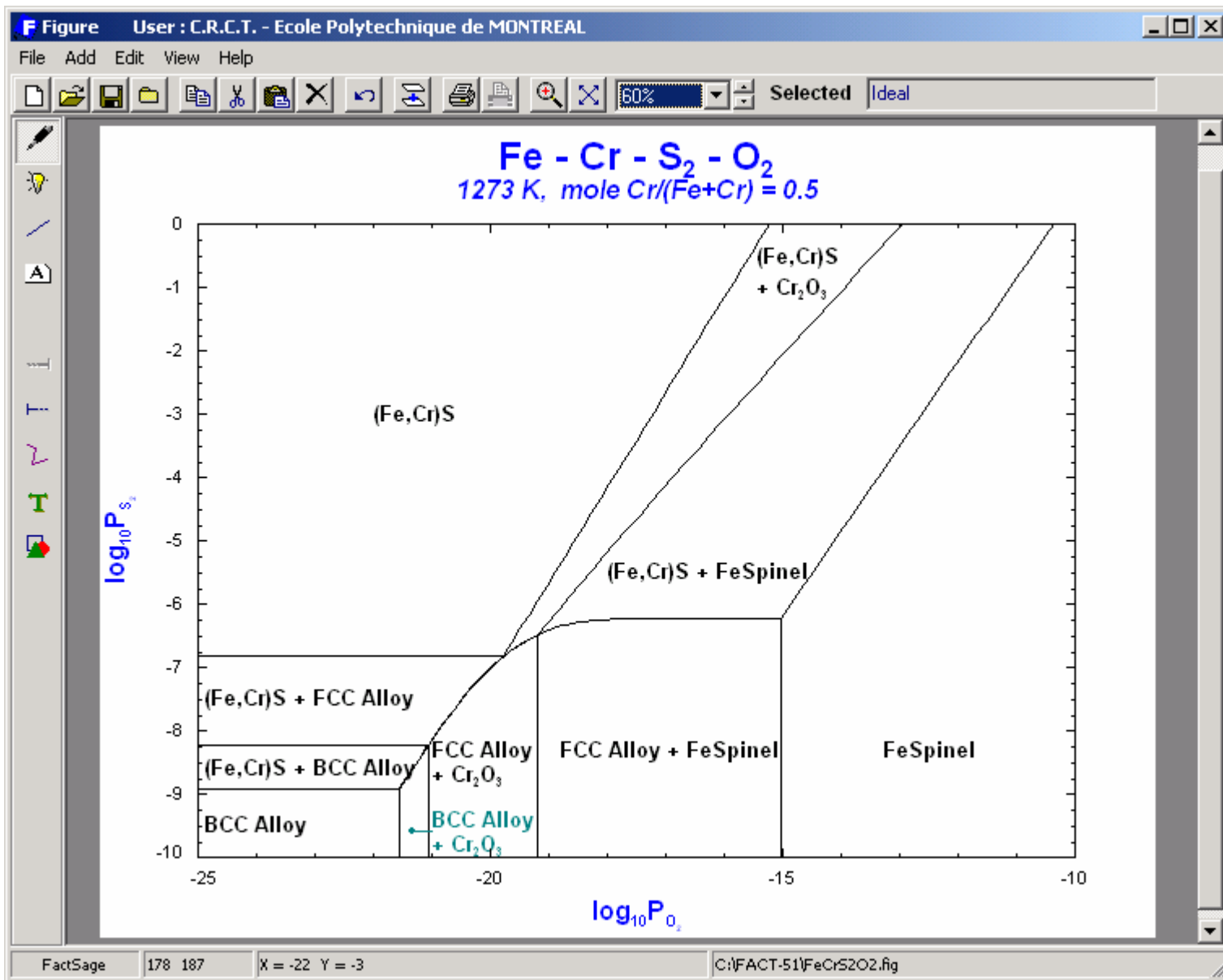
#1. 0 Fe + 1 Cr = constant

1 Fe + 1 Cr = 0.5

Cancel

OK

# Predominance area diagram: Fe-Cr-S<sub>2</sub>-O<sub>2</sub> System, graphical output



# A quaternary isopleth diagram

The following three slides show how the calculation of a **quaternary isopleth** diagram is **prepared and executed**.

Furthermore, the use of the **Point Calculation option** is demonstrated. The resulting equilibrium table is shown and explained.

As an example the **Fe-Cr-V-C** system is used.

# Fe-Cr-V-C system at 1.5 wt% Cr and 0.1 wt% V: **input**

1° **Entry** of the components  
(done in the **Components** window)

- 2° **Definition** of the variables:
- **3 compositions (1 axis)**
  - **600°C < T < 1000°C**
  - **P = 1 atm**

**Components (4)**  
(gram) Fe + Cr + V + C

**Products**

	+	Base-Phase	Full Name
	I	SGSL-FCC	FCC
	I	SGSL-BCC	BCC
	+	SGSL-CEME	CEMENTITE
	+	SGSL-M7C3	M(7)C(3)
	+	SGSL-M23C6	M(23)C(6)

**Variables**

T(C)	Cr/(Fe+Cr+V+C)	V/(Fe+Cr+V+C)	C/(Fe+Cr+V+C)
600 1000	0.015	0.001	0 0.01

T(C) vs C/(Fe+Cr+V+C)

Calculate >>

- 3° **Selection** of the products:
- **5 solid solutions** (including 2 with possible miscibility gap)

4° **Computation** of the phase diagram

**Variables**  
composition 3

**T and P**  
Temperature: T(C) Y-axis, 600 to 1000  
Pressure: P(atm) constant

**Compositions (mass)**

#1: 0 Fe + 1 Cr + 0 V + 0 C = constant  
1 Fe + 1 Cr + 1 V + 1 C = 0.015

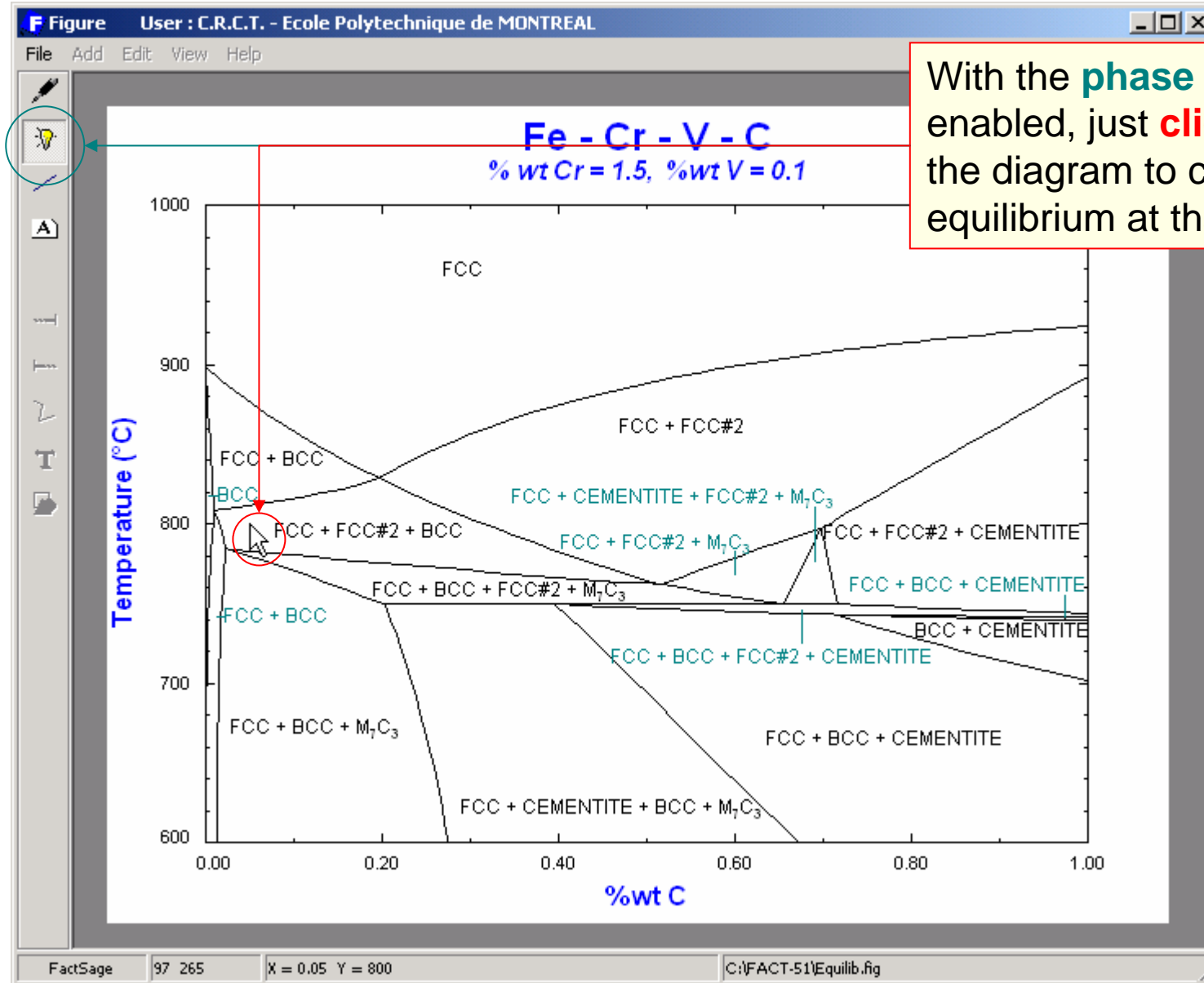
#2: 0 Fe + 0 Cr + 1 V + 0 C = constant  
1 Fe + 1 Cr + 1 V + 1 C = 0.001

#3: 0 Fe + 0 Cr + 0 V + 1 C = X-axis  
1 Fe + 1 Cr + 1 V + 1 C = 0.01 (max)  
0 (min)

Calculate >>



# Fe-Cr-V-C system: graphical output



With the **phase equilibrium mode** enabled, just **click** at any point on the diagram to calculate the equilibrium at that point.

# Fe-Cr-V-C system: phase equilibrium mode output

Output can be obtained in **FACT** or **ChemSage** format. See **Equilib** Slide Show. Example is for FACT format.

Proportions and compositions of the **FCC** phase (Remember the miscibility gap).  
NOTE: One of the FCC phases is metallic (FCC#1), the other is the  $\text{MeC}_{(1-x)}$  carbide.

Proportion and composition of the **BCC** phase.

```
F Show Results - page 1
File Edit
[Icons]
(gram) Fe + Cr + V + C =

0.60411 gram ( 0.29060E-01 wt.% Cr1C1 SCSLo
+ 1.6702 wt.% Cr1Va1 SCSLo
+ 1.6589 wt.% Fe1C1 SCSLo
+ 96.592 wt.% Fe1Va1 SCSLo
+ 0.85663E-03 wt.% V1C1 SCSLo
+ 0.49042E-01 wt.% V1Va1 SCSLo)
(799.38 C, 1 atm, FCC#1)
Mole fraction of sublattice constituents in FCC#1
Cr 0.18223E-01 Stoichiometry = 1.0000
Fe 0.98123
V 0.54617E-03
-----
C 0.13938E-01 Stoichiometry = 1.0000
Va 0.98606

+ 0.54488E-03 gram ( 7.4122 wt.% Cr1C1 SCSLo
+ 0.68214 wt.% Cr1Va1 SCSLo
+ 0.33369 wt.% Fe1C1 SCSLo
+ 0.31112E-01 wt.% Fe1Va1 SCSLo
+ 83.854 wt.% V1C1 SCSLo
+ 7.6872 wt.% V1Va1 SCSLo)
(799.38 C, 1 atm, FCC#2)
Mole fraction of sublattice constituents in FCC#2
Cr 0.79714E-01 Stoichiometry = 1.0000
Fe 0.33850E-02
V 0.91690
-----
C 0.89824 Stoichiometry = 1.0000
Va 0.10176

+ 0.39535 gram ( 0.33016E-03 wt.% Cr1C3 SCSLo
+ 1.1965 wt.% Cr1Va3 SCSLo
+ 0.26466E-01 wt.% Fe1C3 SCSLo
+ 98.704 wt.% Fe1Va3 SCSLo
+ 0.20263E-04 wt.% V1C3 SCSLo
+ 0.72818E-01 wt.% V1Va3 SCSLo)
(799.38 C, 1 atm, BCC#1)
Mole fraction of sublattice constituents in BCC#1
Cr 0.12843E-01 Stoichiometry = 1.0000
Fe 0.98636
V 0.79775E-03
-----
C 0.16295E-03 Stoichiometry = 3.0000
Va 0.99984

+ 0.00000 gram ( 0.33016E-03 wt.% Cr1C3 SCSLo
```

# A ternary isothermal diagram

The following two slides show the input that is needed to define the calculation of a **ternary isothermal phase** diagram.

The example is the system **CaO-Al<sub>2</sub>O<sub>3</sub>-SiO<sub>2</sub>**. The calculated diagram has been **edited using the phase label option**.

# CaO-Al<sub>2</sub>O<sub>3</sub>-SiO<sub>2</sub> ternary phase diagram: **input**

1° **Entry** of the components  
(done in the **Components** window)

- 2° **Definition** of the variables:
- **2 Compositions** (by default)
  - **T = 1573K**
  - **P = 1 atm**
  - **Triangular plot**

**F Menu - Phase Diagram**

File Units Parameters Variables Help

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

Components (3)

(gram) CaO + Al<sub>2</sub>O<sub>3</sub> + SiO<sub>2</sub>

Products

Compound species:

- gas  ideal  real 0
- liquid  0
- aqueous  0
- solid  44
- suppress duplicates

Species: 44

Target: - none -

Estimate T(K): 1000

Mass(g): 0

Solution species:

+	Base-Phase	Full Name
+	FACT-SLAG	Slag

Legend: + - selected

show  all  selected

species: 3 solutions: 1

Clear

Custom Solutions:

- fixed activities
- ideal solutions
- activity coefficients

Details ...

Pseudonyms:

apply  List ...

include molar volumes

Total Species (max 692) 47

Total Solutions (max 30) 1

Default

Variables

T(C)	CaO/(CaO+Al <sub>2</sub> O <sub>3</sub> )	Al <sub>2</sub> O <sub>3</sub> /(CaO+Al <sub>2</sub> O <sub>3</sub> )		
1600	0.1	0.1		

A = CaO, B = SiO<sub>2</sub>, C = Al<sub>2</sub>O<sub>3</sub>

Phase Diagram

Calculate >>

- 3° **Selection** of the products:
- **Solid**
  - **1 solution phase (FACT-SLAG)**

4° **Computation** of the **ternary phase diagram** as a **triangular plot**

**F Variables: CaO-Al<sub>2</sub>O<sub>3</sub>-SiO<sub>2</sub> - vs -**

Variables

composition

log10(a)

RTln(a)

Y steps: 5

X steps: 5

Next >>

T and P

Temperature:  T(C) constant  1/TK 1600

Pressure:  P(atm) constant  log P 1

Compositions (mass)

#1.  CaO +  Al<sub>2</sub>O<sub>3</sub> +  SiO<sub>2</sub> = A-Corner

CaO +  Al<sub>2</sub>O<sub>3</sub> +  SiO<sub>2</sub> = 1 (max)

CaO +  Al<sub>2</sub>O<sub>3</sub> +  SiO<sub>2</sub> = C-Corner

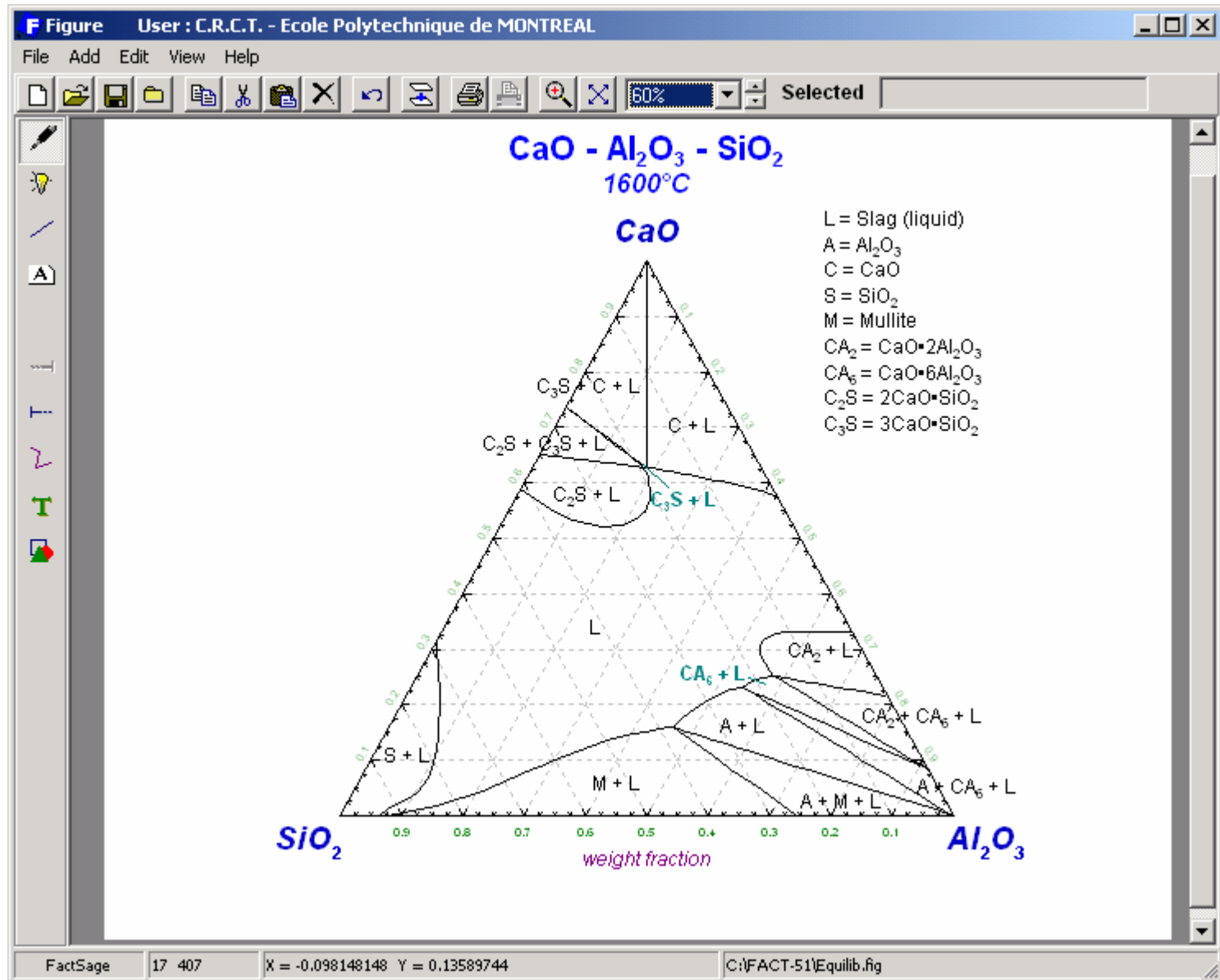
CaO +  Al<sub>2</sub>O<sub>3</sub> +  SiO<sub>2</sub> = 1 (max)

CaO +  Al<sub>2</sub>O<sub>3</sub> +  SiO<sub>2</sub> = B-Corner

CaO +  Al<sub>2</sub>O<sub>3</sub> +  SiO<sub>2</sub> = 1 (max)

Cancel OK

# CaO-Al<sub>2</sub>O<sub>3</sub>-SiO<sub>2</sub> ternary phase diagram: graphical output



FactSage

17 407

X = -0.098148148 Y = 0.13589744

C:\FACT-51\Equilib.fig

# Using Zero Phase Fraction lines in graphs

**Zero Phase Fraction (ZPF) lines** are essential for the calculation and interpretation of the resulting phase diagrams.

ZPF lines constitute the **set of phase boundaries** in a phase diagram that depict the **outer edge of appearance (zero phase fraction)** of a particular phase. When crossing the line the phase either appears or disappears depending on the direction.

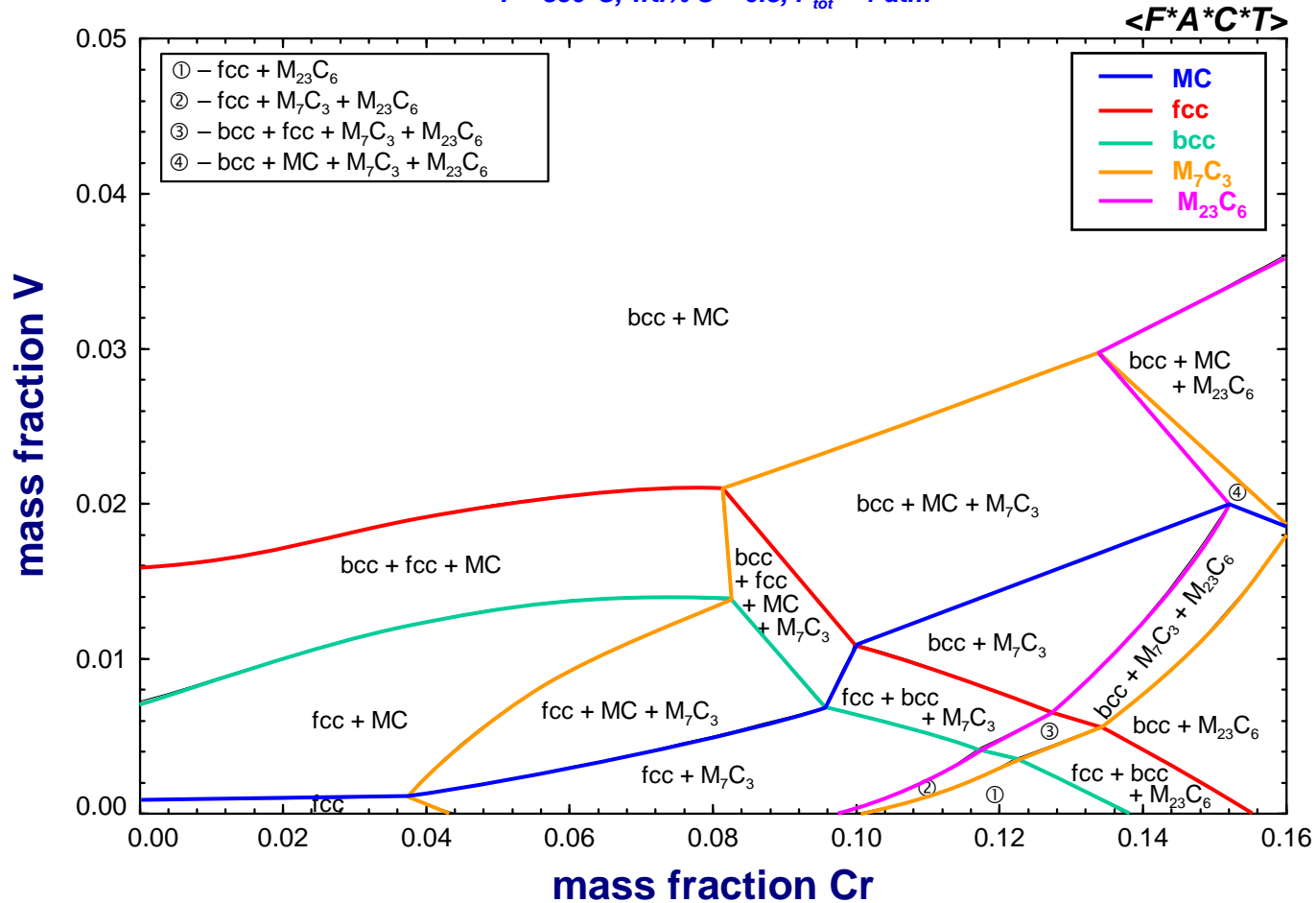
The following three slides show examples of calculated phase diagrams with the ZPF lines marked in color. [Slides 13.1 and 13.2](#) are easy to understand since they both have at least one compositional axis.

Note however, that it is also possible to mark ZPF lines in a **predominance area type diagram** ([slide 13.3](#)) although no phase amounts are given in this type of diagram. As a result the phase boundaries are marked with two colors since the lines themselves are the two phase «fields», i.e. **each line is a boundary for TWO phases**.

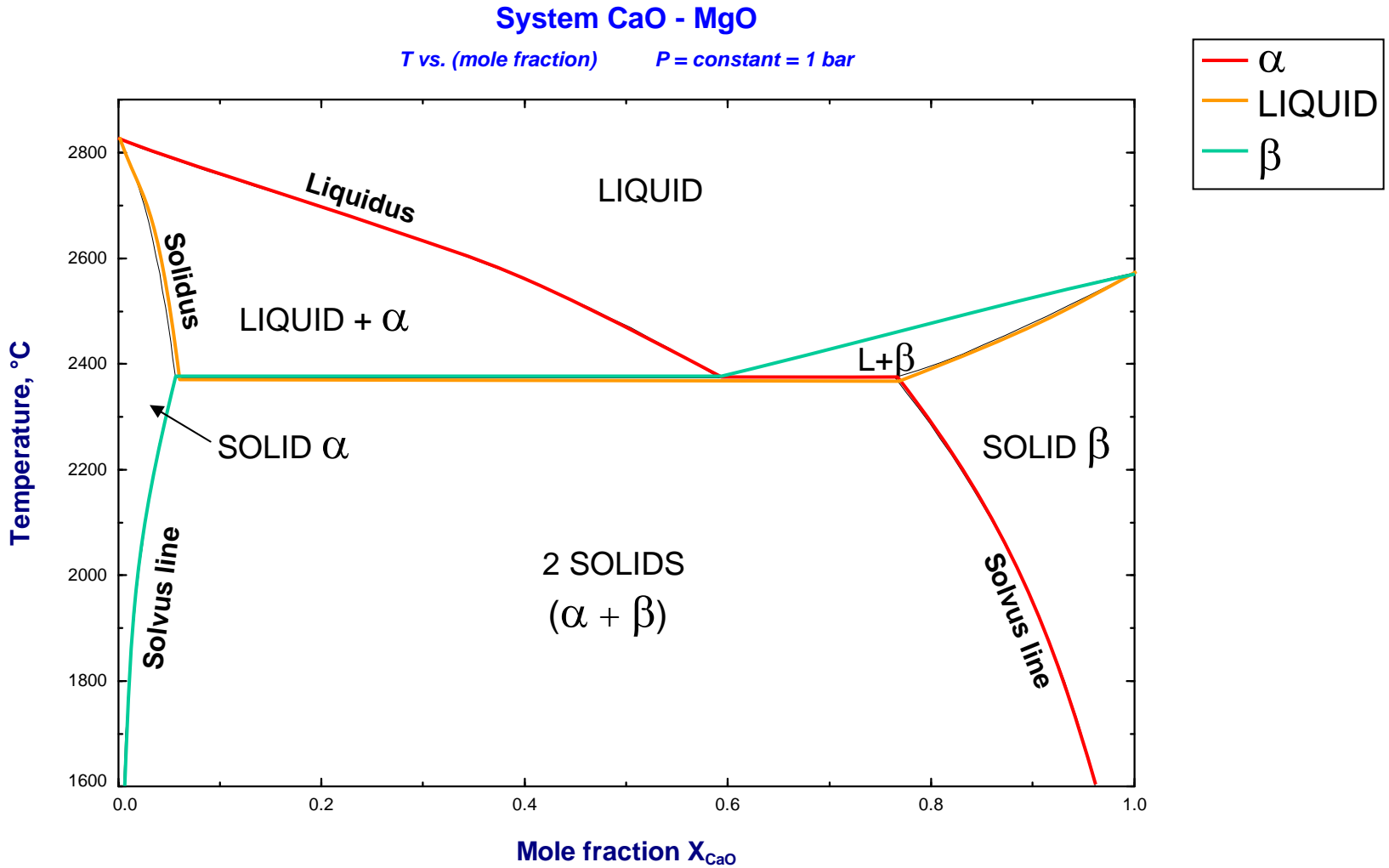
# Zero Phase Fraction (ZPF) Lines

## Fe - Cr - V - C System

$T = 850^{\circ}\text{C}$ , wt.% C = 0.3,  $P_{\text{tot}} = 1 \text{ atm}$

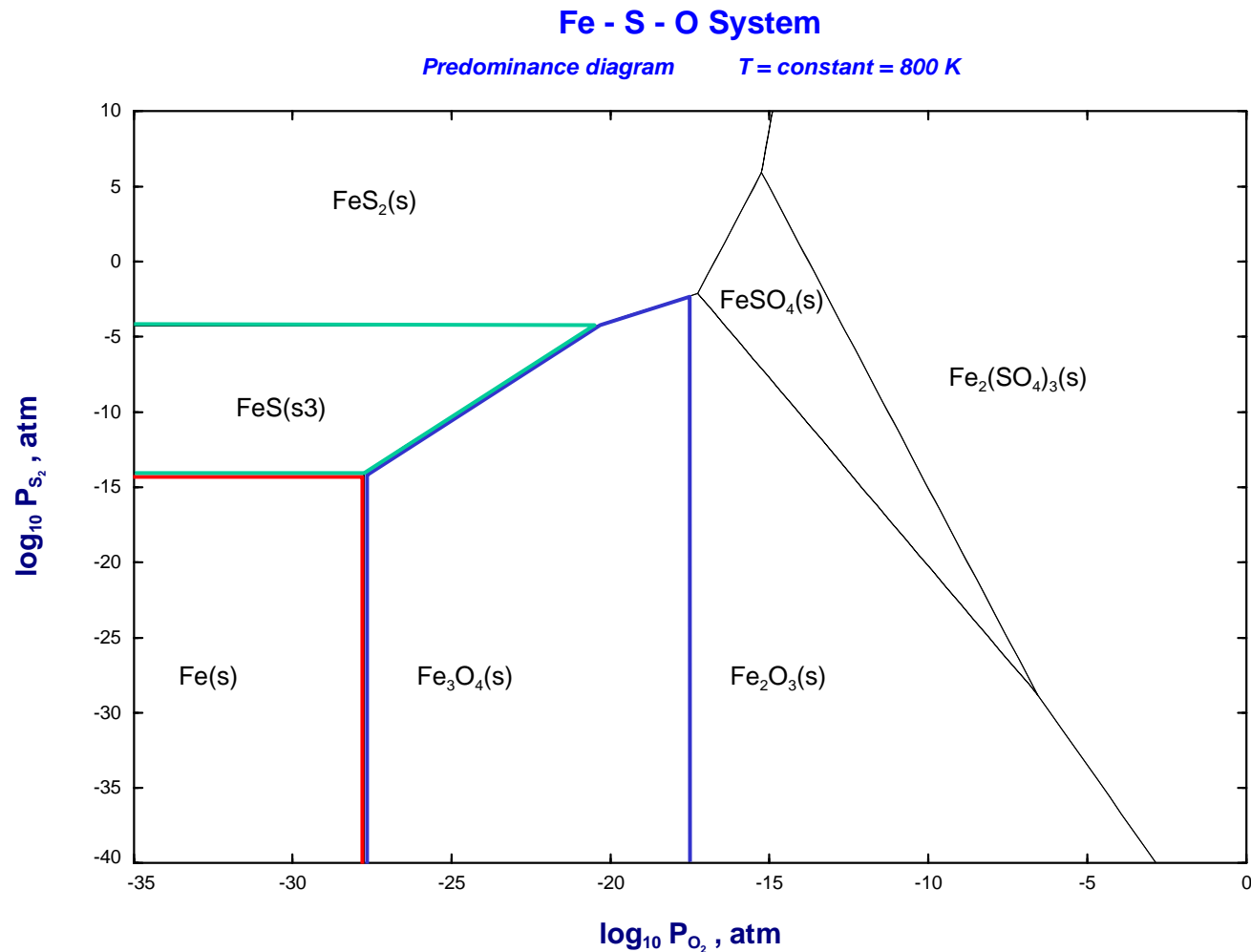


# Zero Phase Fraction (ZPF) Lines





# Fe - S - O Predominance diagram (ZPF lines)



# Generalized rules for phase diagrams

The following two slides show the **rules for the choice of axes variables** such that **proper phase diagrams** result from the calculation.

The basic relationship for these rules is given by the **Gibbs-Duhem equation** which interrelates a set of **potential variables** with their respective **conjugate extensive variables**.

**Only one variable from each pair** may be used in the definition of the axes variables. If **extensive properties** are to be used **ratios** of these need to be employed in the definition of the axes variables.

# N-Component System (A-B-C-...-N)

## Extensive variable

$q_i$

$S$

$V$

$n_A$

$n_B$

$\cdot$

$\cdot$

$\cdot$

$n_N$

## Corresponding potential

$$\phi_i = \left( \frac{\partial U}{\partial q_i} \right)_{q_j}$$

$T$

$-P$

$\mu_A$

$\mu_B$

$\cdot$

$\cdot$

$\cdot$

$\mu_N$

$$dU = TdS - PdV + \sum \mu_i dn_i = \sum \phi_i dq_i$$

**Gibbs-Duhem:**  $SdT + VdP + \sum n_i d\mu_i = \sum q_i d\phi_i = 0$

## N-component system

- (1) Choose  $n$  potentials:  $\phi_1, \phi_2, \dots, \phi_n$  ( $n \leq N + 1$ )
- (2) From the non-corresponding extensive variables ( $q_{n+1}, q_{n+2}, \dots$ ), form  $(N+1-n)$  independent ratios ( $Q_{n+1}, Q_{n+2}, \dots, Q_{N+1}$ ).

Example:

$$Q_i = \frac{q_i}{\sum_{j=n+1}^{N+1} q_j} \quad (n+1 \leq i \leq N+1)$$

$[\phi_1, \phi_2, \dots, \phi_n; Q_{n+1}, Q_{n+2}, \dots, Q_{N+1}]$  are then the  $(N+1)$  variables of which 2 are chosen as axes and the remainder are held constant.

# Using the **rules for classical cases**

The following four slides show how the rules outlined above are employed for the selection of proper axes in the case of

the **T vs x diagram** of the system **CaO-MgO**

and

the **log P(S<sub>2</sub>) vs log P(O<sub>2</sub>) diagram** for the system **Fe-Cr-S<sub>2</sub>-O<sub>2</sub>**.

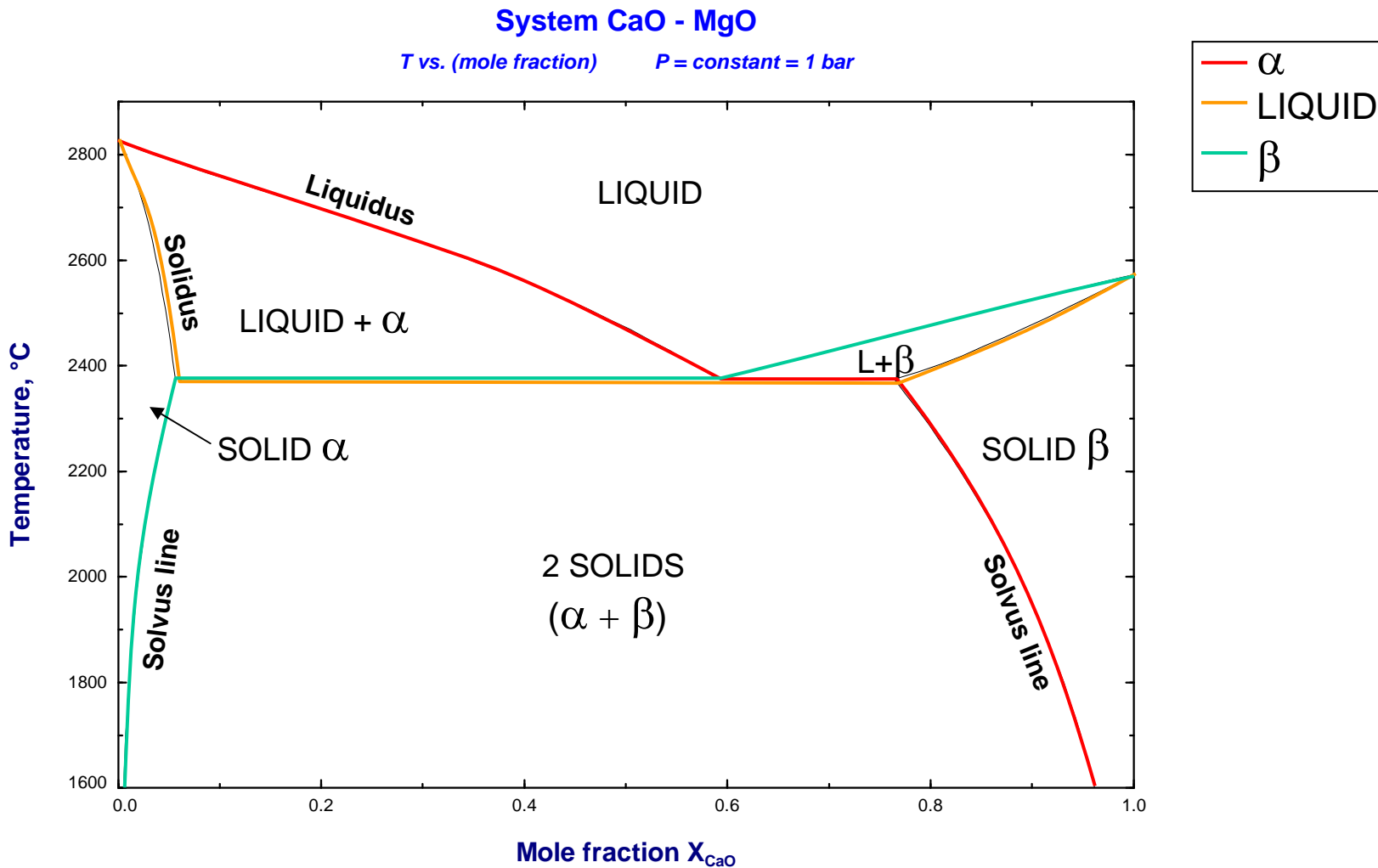
The calculated phase diagrams are also shown.

# MgO-CaO Binary System

$S$	$T$
$V$	$-P$
$n_{MgO}$	$\mu_{MgO}$
$n_{CaO}$	$\mu_{CaO}$

$\phi_1 = T$	<i>y-axis</i>
$\phi_2 = -P$	<i>constant</i>
$q_3 = n_{MgO}$	} $Q_3 = \frac{n_{CaO}}{(n_{MgO} + n_{CaO})}$
$q_4 = n_{CaO}$	

# T vs x diagram: CaO-MgO System, graphical output



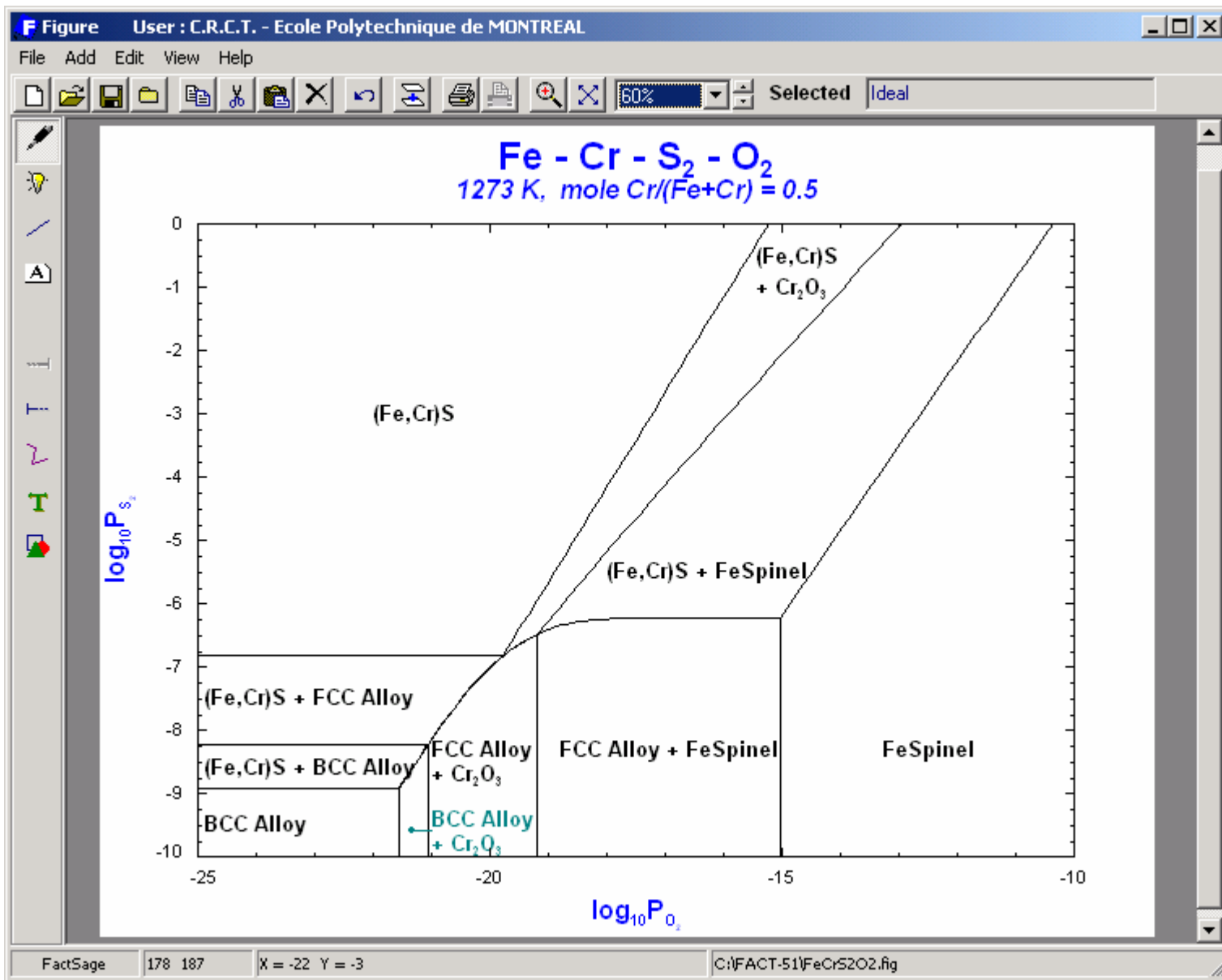
# Fe - Cr - S<sub>2</sub> - O<sub>2</sub> System

$S$	$T$
$V$	$-P$
$n_{O_2}$	$\mu_{O_2}$
$n_{S_2}$	$\mu_{S_2}$
$n_{Fe}$	$\mu_{Fe}$
$n_{Cr}$	$\mu_{Cr}$

$\phi_1 = T$	<i>constant</i>
$\phi_2 = -P$	<i>constant</i>
$\phi_3 = \mu_{O_2}$	<i>x-axis</i>
$\phi_4 = \mu_{S_2}$	<i>y-axis</i>
$\left. \begin{array}{l} q_5 = n_{Cr} \\ q_6 = n_{Fe} \end{array} \right\} Q_5 = \frac{n_{Cr}}{n_{Fe}}$	<i>constant</i>



# Predominance area diagram: Fe-Cr-S<sub>2</sub>-O<sub>2</sub> System, graphical output



# Breaking the rules: Diagrams but not phase diagrams

The following three diagrams will show how the «wrong» choice of axes variables, i.e. combinations which are not permitted according to the rules outlined in [slides 14.1 and 14.2](#), leads to diagrams which

(1) are **possible but not permitted** in the input of the phase diagram module, and  
(2) which are **not true phase diagrams** (because a unique equilibrium condition is not necessarily represented at every point).

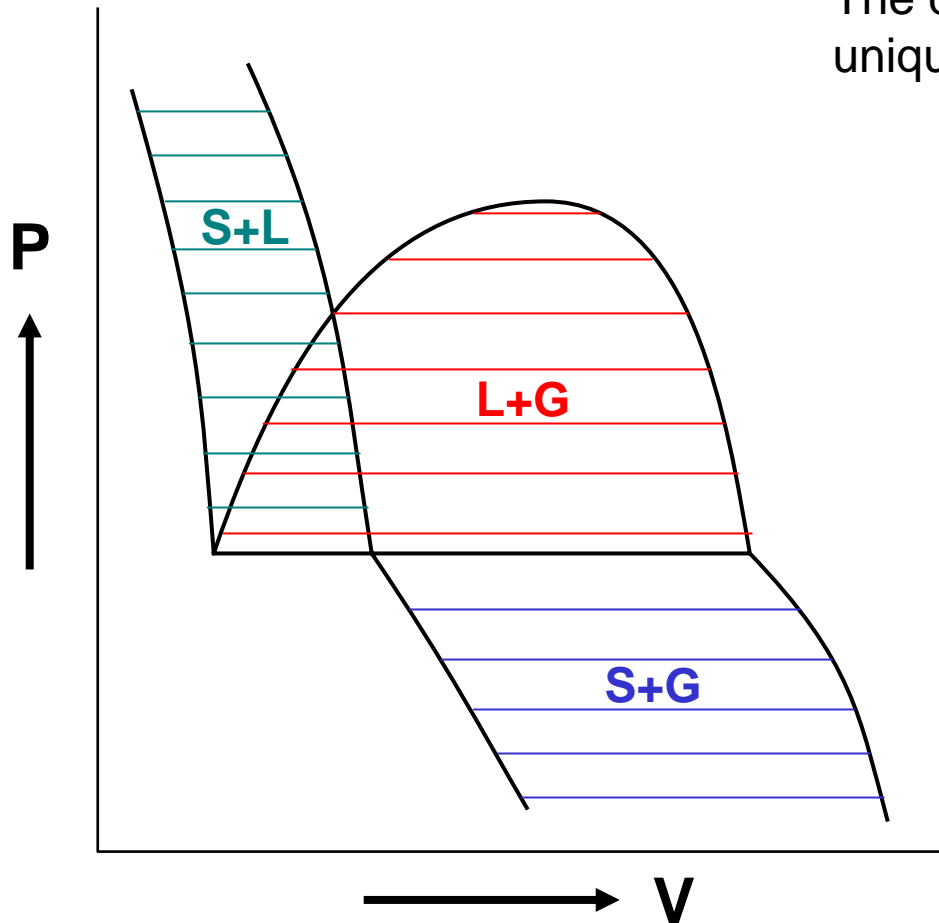
- A simple **one component case** is the P-V diagram for the **water** system with liquid, gas and solid ([Slide 16.1](#)).
- A more complex case is shown for the **ternary system Fe-Cr-C** where one axis is chosen as activity of carbon while the other is mole fraction of Cr. The case shown is not a true phase diagram because of the way the mole fraction of Cr is defined:

The total set of mole numbers, i.e. including the mole number of C, is used. Thus both **the mole number and the activity of carbon** are being used for the axes variables. **This is NOT permitted for true phase diagrams.**

# Pressure vs. Volume diagram for $H_2O$

This is **NOT** a true phase diagram.

The double marked area can not be uniquely attributed to one set of phases.



# Fe - Cr - C System

$S$	$T$
$V$	$-P$
$n_C$	$\mu_C$
$n_{Fe}$	$\mu_{Fe}$
$n_{Cr}$	$\mu_{Cr}$

$\phi_1 = T$	<i>constant</i>
$\phi_2 = -P$	<i>constant</i>
$\phi_3 = \mu_C \rightarrow a_C$	<i>x-axis</i>
$Q_4 = \frac{n_{Cr}}{(n_{Fe} + n_{Cr} + n_C)}$	<b>(NOT OK)</b>
$Q_4 = \frac{n_{Cr}}{(n_{Fe} + n_{Cr})}$	<b>(OK)</b> <i>y-axis</i>

Requirement:  $\frac{dQ_j}{dq_i} = 0$  for  $i \leq 3$

# Fe - Cr - C system, $T = 1300\text{ K}$ , $X_{\text{Cr}} = n_{\text{Cr}} / (n_{\text{Fe}} + n_{\text{Cr}} + n_{\text{C}})$ vs $a_{\text{C}}$ (carbon activity)

This is **NOT** a true phase diagram.

The areas with the «**swallow tails**» cannot be uniquely attributed to one set of phases.

