What‘s new in FactSage 7.0
A brief overview

K. Hack

GTT Users Meeting July 2014

Major new features

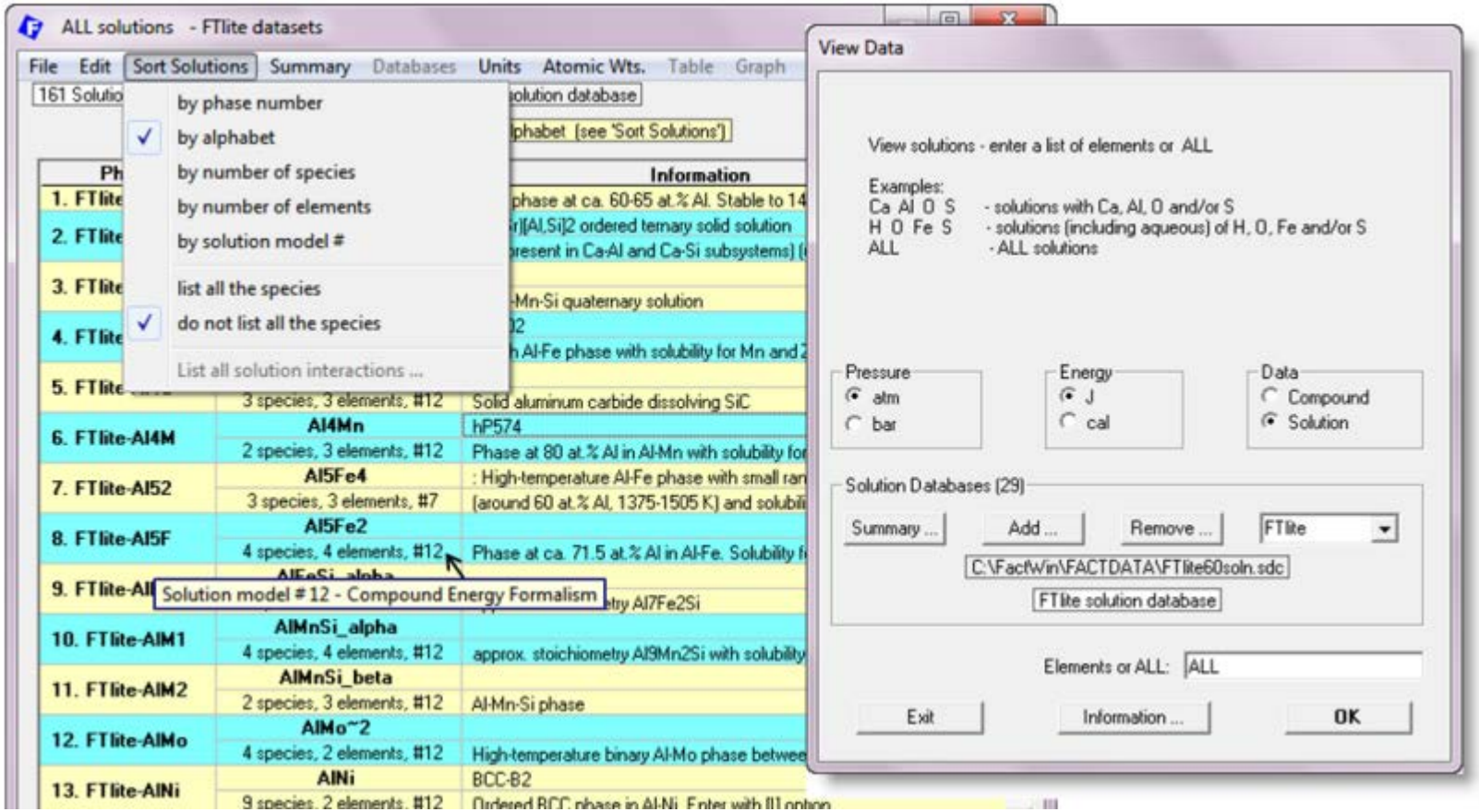
- Extended Slide Show on Steel Applications
- Additional commands in Macro Language
- Modifications in many databases
- New SGTE Solution database
- „ALL“ feature for Solution Databases in View Data module
- New Solution module
- Iso-bar and Iso-activity lines in Phase Diagram module

New SGTE Solution database

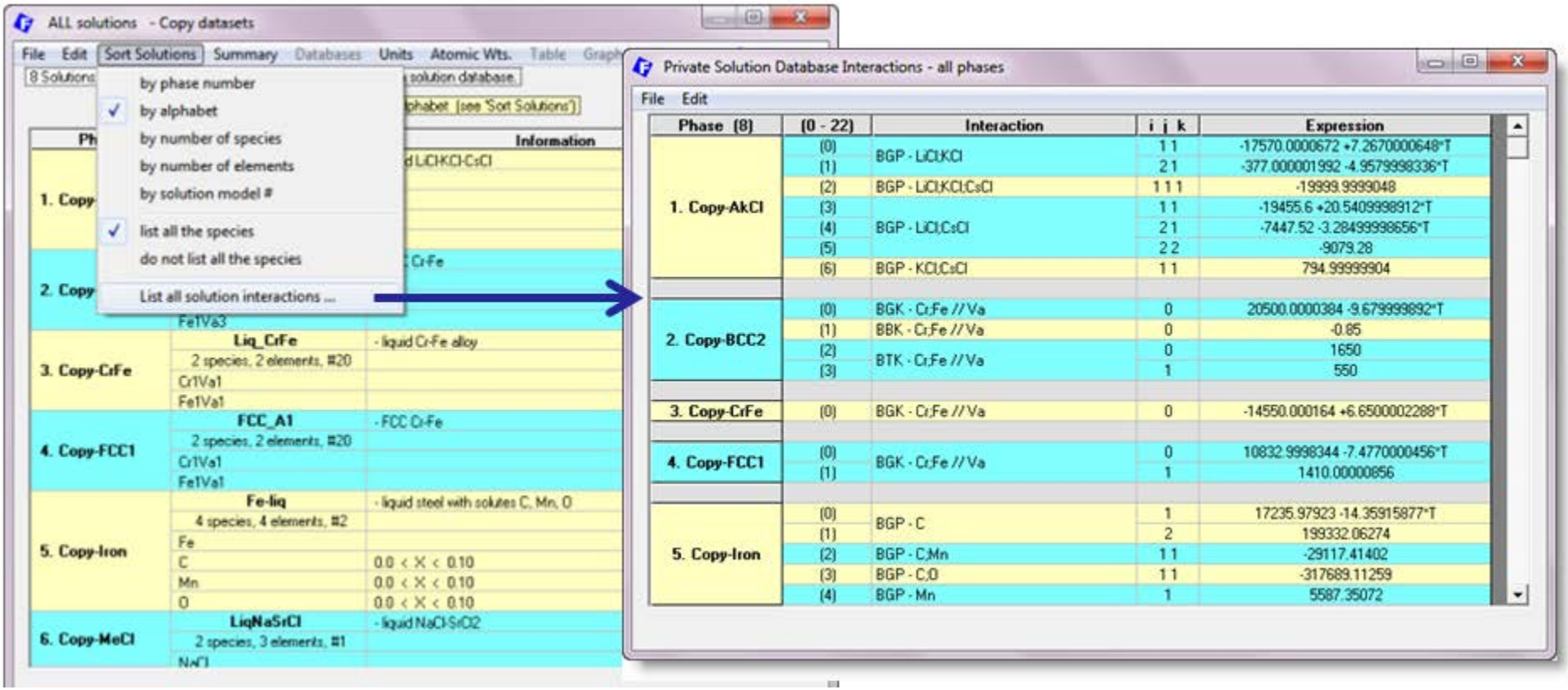
- Conversion of the new database in very close co-operation with the SGTE Solution database manager

- 583 binary systems
- 127 ternary systems → 669 isotherms
- 8 complete quaternary systems

ALL feature now also for Solution databases available



… continued:


ALL solutions - Copy datasets
File Edit Sort Solutions Summary Databases Units Atomic Wts. Table Graph
8 Solutions
by phase number
by alphabet
by number of species
by number of elements
by solution model #
list all the species
do not list all the species
List all solution interactions ...
Information
1. Copy-
2. Copy-
3. Copy-CrFe
Liq_CrFe
- liquid Cr-Fe alloy
2 species, 2 elements, #20
Cr1Va1
Fe1Va1
4. Copy-FCC1
FCC_A1
- FCC Cr-Fe
5. Copy-Iron
Fe-liq
- liquid steel with solutes C, Mn, O
4 species, 4 elements, #2
Fe
C 0.0 < X < 0.10
Mn 0.0 < X < 0.10
O 0.0 < X < 0.10
6. Copy-MeCl
LiqNaSrCl
- liquid NaCl-SrCl2
2 species, 3 elements, #1
Private Solution Database Interactions - all phases
File Edit
Phase (8) | (0 - 22) | Interaction | i j k | Expression
1. Copy-AkCl
(0) BGP - LiCl,KCl 1 1 -17570.0000672 +7.2670000648*T
(1) 2 1 -377.00001992 -4.9579998336*T
(2) BGP - LiCl,KCl,CsCl 1 1 1 -19999.9999048
(3) 1 1 -19455.6 +20.5409998912*T
(4) BGP - LiCl,CsCl 2 1 -7447.52 -3.28499998656*T
(5) 2 2 -9079.28
(6) BGP - KCl,CsCl 1 1 794.99999904
2. Copy-BCC2
(0) BGK - Cr,Fe // Va 0 20500.0000384 -9.679999892*T
(1) BBK - Cr,Fe // Va 0 -0.65
(2) BTK - Cr,Fe // Va 0 1650
(3) 1 550
3. Copy-CrFe
(0) BGK - Cr,Fe // Va 0 -14550.000164 +6.6500002288*T
4. Copy-FCC1
(0) BGK - Cr,Fe // Va 0 10832.9998344 -7.4770000456*T
(1) 1 1410.00000856
5. Copy-Iron
(0) BGP - C 1 17235.97923 -14.35915877*T
(1) 2 199332.06274
(2) BGP - C,Mn 1 1 -29117.41402
(3) BGP - C,O 1 1 -317689.11259
(4) BGP - Mn 1 5587.35072

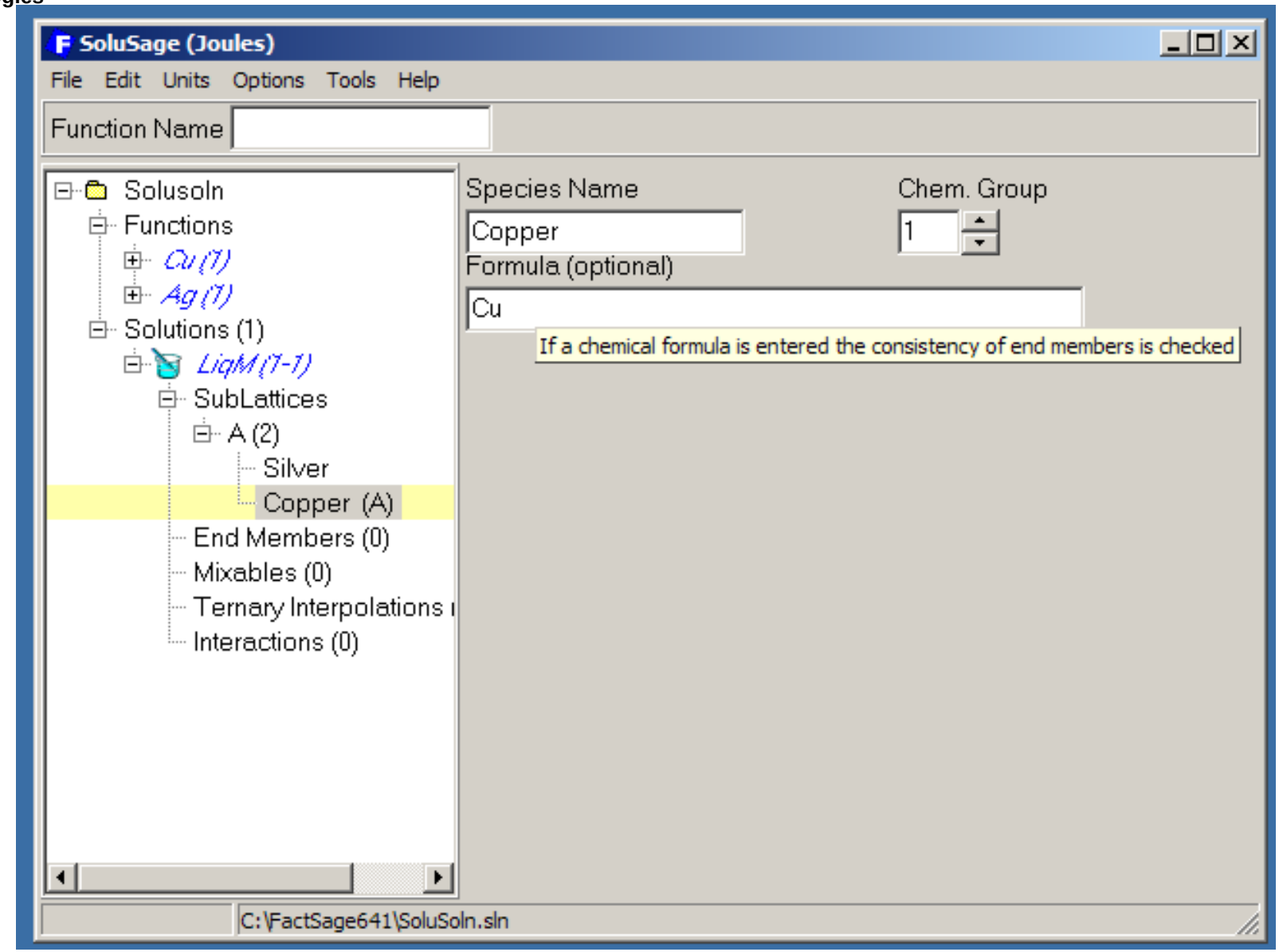
New Solution module (for private solution databases)

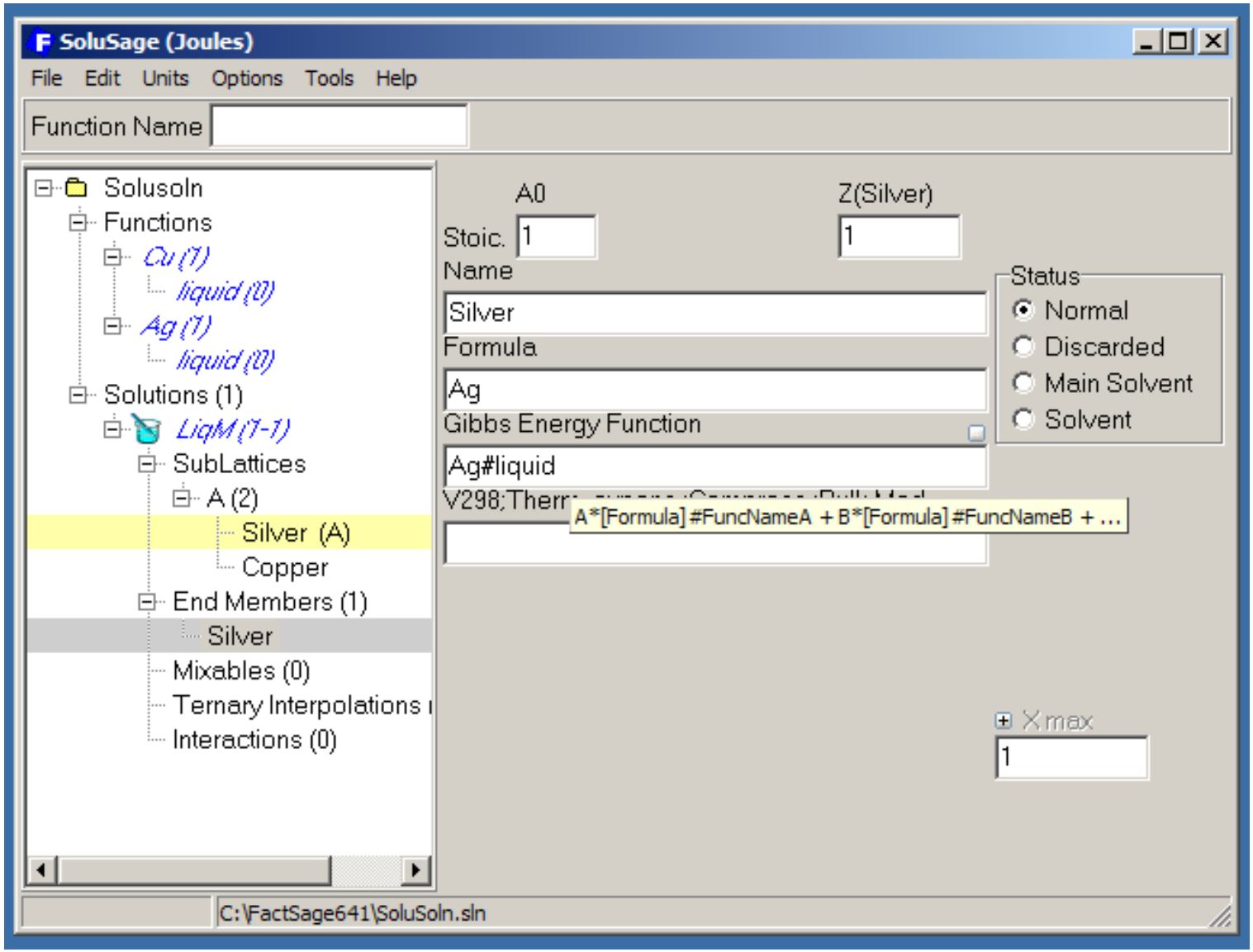
- Interaction with Compound module for the definition of phase constituents and functions
- All solution models available for user input, including aqueous, various polynomial approaches with selectable ternary interactions, several variants of the quasi-chemical model, compound energy formalism (up to 5 sublattices)
- Use of „full text“ expressions for temperature dependent terms

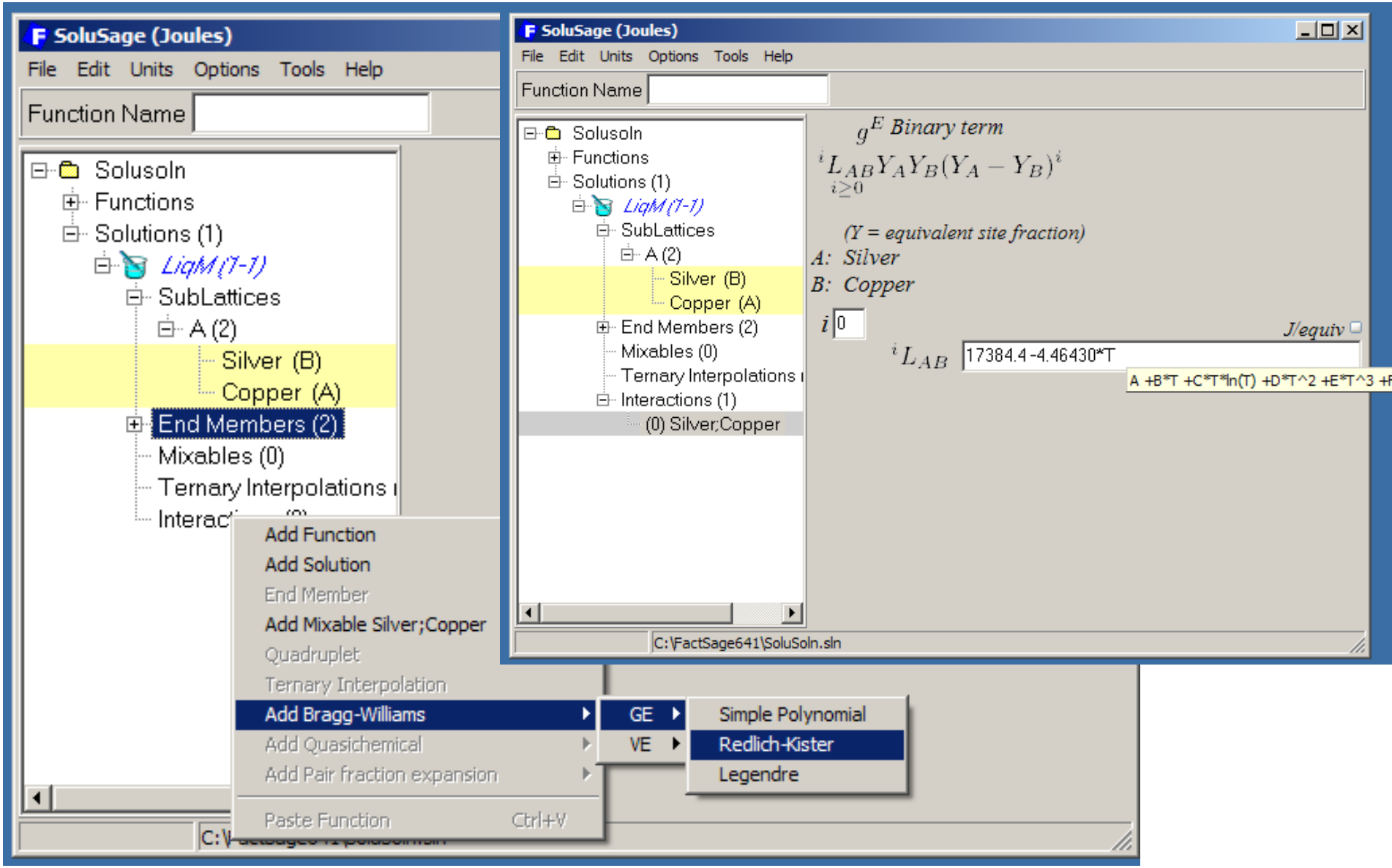
A short view on the new Solution module

- A new private database contains
  - Functions
  - Phases
    - Sublattices (with species)
      - Constituents (end members made from species)
    - Interactions
      - Binary
      - Ternary
      - … higher order terms

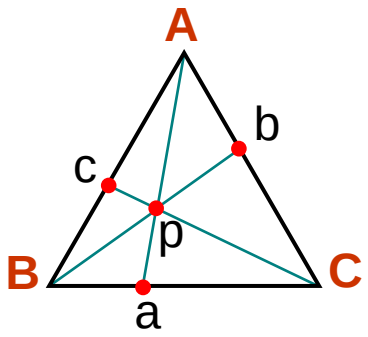
Additionally, magnetic terms, volume data, etc. can also be incorporated in a database.


SoluSage (Joules)
File
Edit
Units
Options
Tools
Help
Function Name
Solusoln
Functions
Cu (T)
Ag (T)
Solutions (1)
LiqM (T-1)
SubLattices
A (2)
Silver
Copper (A)
End Members (0)
Mixables (0)
Ternary Interpolations
Interactions (0)
Species Name
Copper
Chem. Group
1
Formula (optional)
Cu
If a chemical formula is entered the consistency of end members is checked
C:\FactSage641\SoluSoln.sln

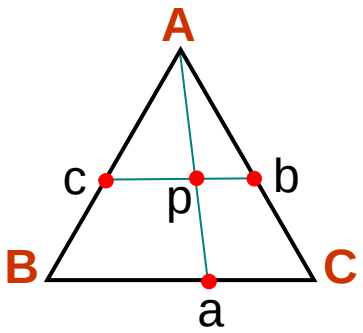

SoluSage (Joules)
File Edit Units Options Tools Help
Function Name
Solusoln
Functions
Cu (1)
liquid (0)
Ag (1)
liquid (0)
Solutions (1)
LiqM (1-1)
SubLattices
A (2)
Silver (A)
Copper
End Members (1)
Silver
Mixables (0)
Ternary Interpolations
Interactions (0)
A0
Z(Silver)
Stoic.
1
1
Name
Silver
Formula
Ag
Gibbs Energy Function
Ag#liquid
A*[Formula]#FuncNameA + B*[Formula]#FuncNameB + ...
Status
Normal
Discarded
Main Solvent
Solvent
Xmax
1
C:\FactSage641\SoluSoln.sln


SoluSage (Joules)
File Edit Units Options Tools Help
Function Name
SoluSoln
Functions
Solutions (1)
LiqM(T-1)
SubLattices
A (2)
Silver (B)
Copper (A)
End Members (2)
Mixables (0)
Ternary Interpolations
Interac
Add Function
Add Solution
End Member
Add Mixable Silver;Copper
Quadruplet
Ternary Interpolation
Add Bragg-Williams
Add Quasichemical
Add Pair fraction expansion
Paste Function Ctrl+V
GE
VE
Simple Polynomial
Redlich-Kister
Legendre
SoluSage (Joules)
File Edit Units Options Tools Help
Function Name
SoluSoln
Functions
Solutions (1)
LiqM(T-1)
SubLattices
A (2)
Silver (B)
Copper (A)
End Members (2)
Mixables (0)
Ternary Interpolations
Interactions (1)
(0) Silver;Copper
g^E Binary term
${}^iL_{AB} Y_A Y_B (Y_A - Y_B)^i$
$i \geq 0$
(Y = equivalent site fraction)
A: Silver
B: Copper
i 0
J/equiv
${}^iL_{AB}$ 17384.4 -4.46430*T
A +B*T +C*T*ln(T) +D*T^2 +E*T^3 +F
C:\FactSage641\SoluSoln.sln

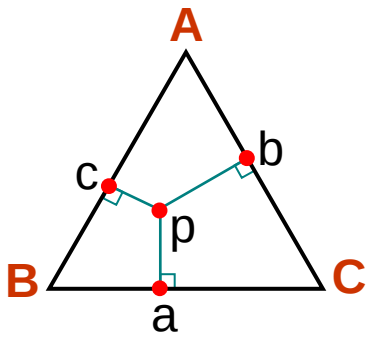
Ternary terms



"All Kohler"

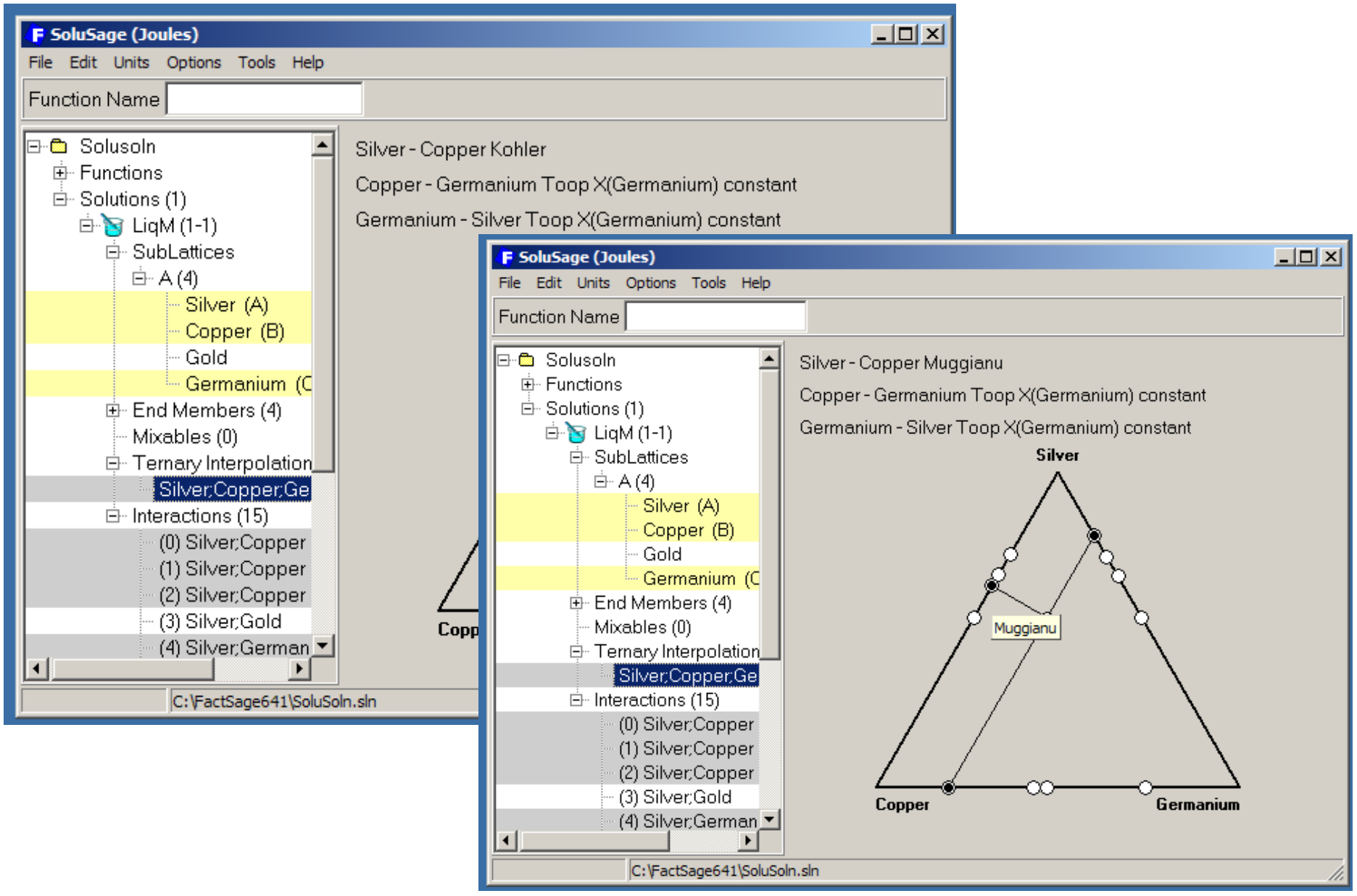


"Kohler/Toop (X_A = constant)"

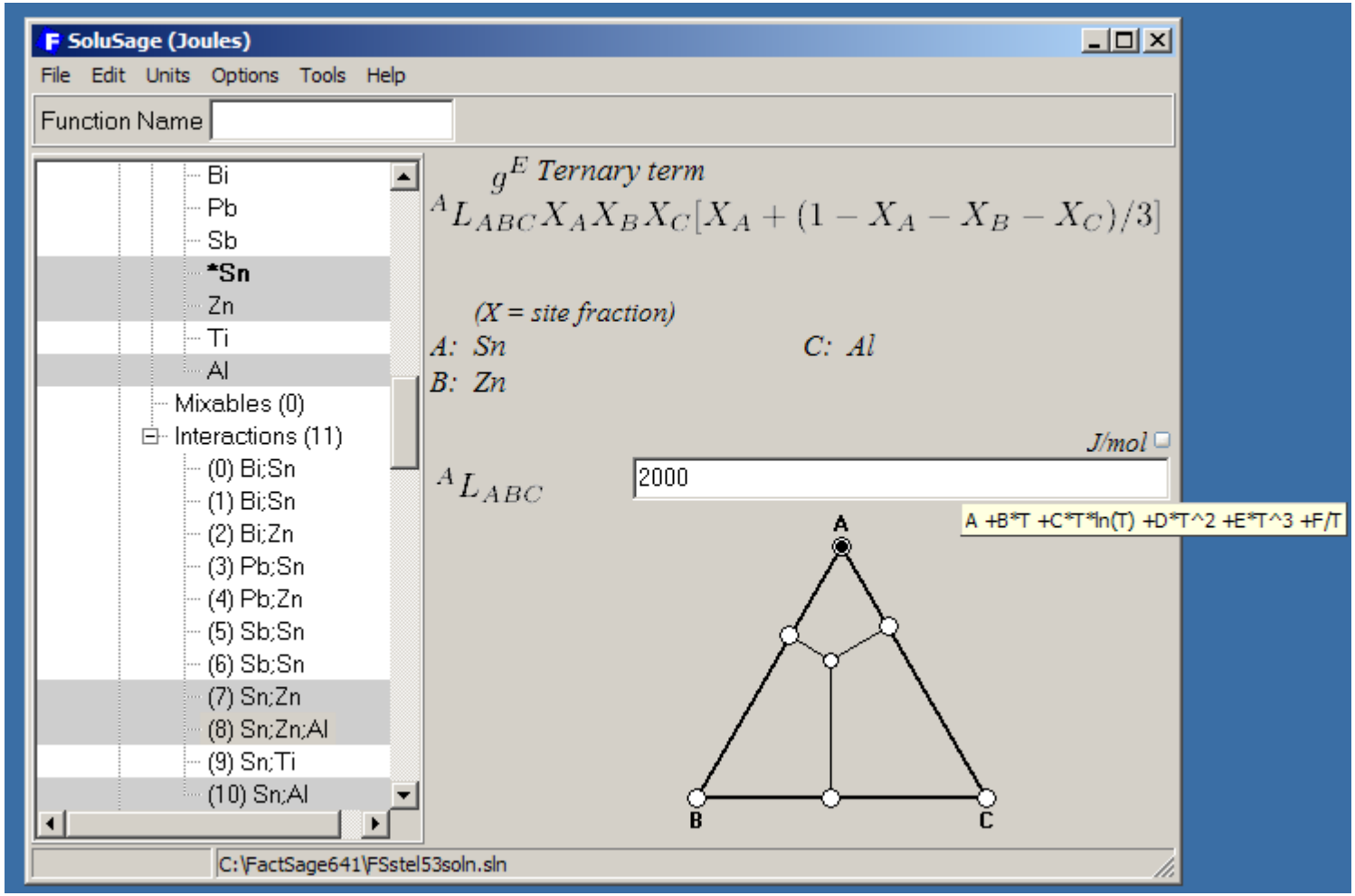


"All Muggianu"

- Each component of a solution phase is assigned a **"chemical group number"** (1, 2, 3…). (Usually, components which are chemically similar are assigned the same group number.)
- If A, B and C are all members of the same group, or are members of three different groups, then the **"All Kohler"** configuration is the default.
- If B and C are in the same group while A is in a different group, then the **"Kohler/Toop (X_A = constant)"** configuration is the default.
- If one or more of A, B or C is in group "0", then **"All Muggianu"** is the default configuration.
- However, for any ternary sub-system, the **default configuration can be over-written**.


SoluSage (Joules)
File Edit Units Options Tools Help
Function Name
Solusoln
Functions
Solutions (1)
LiqM (1-1)
SubLattices
A (4)
Silver (A)
Copper (B)
Gold
Germanium (C
End Members (4)
Mixables (0)
Ternary Interpolation
Silver;Copper;Ge
Interactions (15)
(0) Silver;Copper
(1) Silver;Copper
(2) Silver;Copper
(3) Silver;Gold
(4) Silver;German
Silver - Copper Kohler
Copper - Germanium Toop X(Germanium) constant
Germanium - Silver Toop X(Germanium) constant
C:\FactSage641\SoluSoln.sln
SoluSage (Joules)
File Edit Units Options Tools Help
Function Name
Solusoln
Functions
Solutions (1)
LiqM (1-1)
SubLattices
A (4)
Silver (A)
Copper (B)
Gold
Germanium (C
End Members (4)
Mixables (0)
Ternary Interpolation
Silver;Copper;Ge
Interactions (15)
(0) Silver;Copper
(1) Silver;Copper
(2) Silver;Copper
(3) Silver;Gold
(4) Silver;German
Silver - Copper Muggianu
Copper - Germanium Toop X(Germanium) constant
Germanium - Silver Toop X(Germanium) constant
Silver
Muggianu
Copper
Germanium
C:\FactSage641\SoluSoln.sln

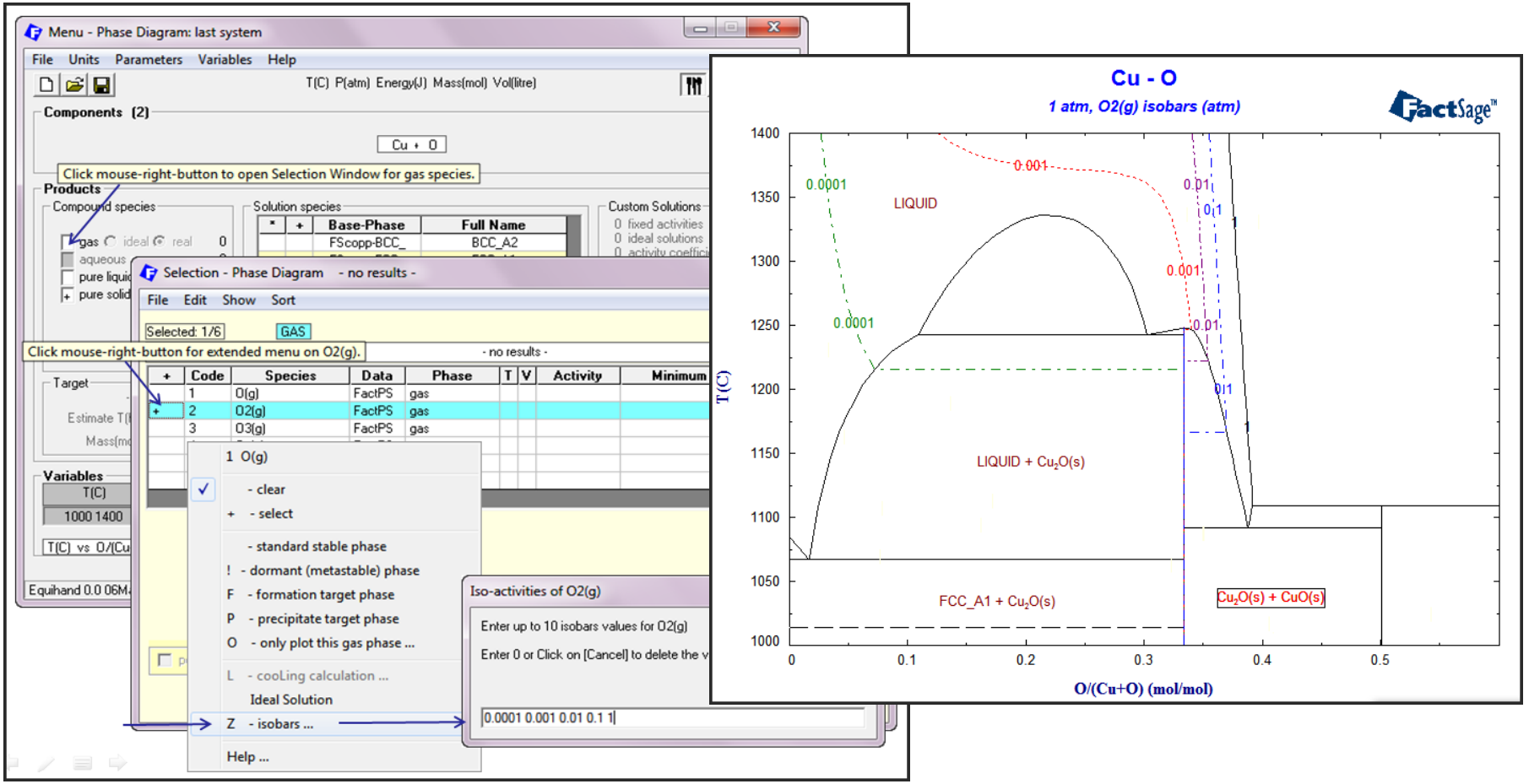
Muggianu term



… etc. … etc.

- All mixing models are now available for use in the Solution module

Iso-bar and Iso-activity lines



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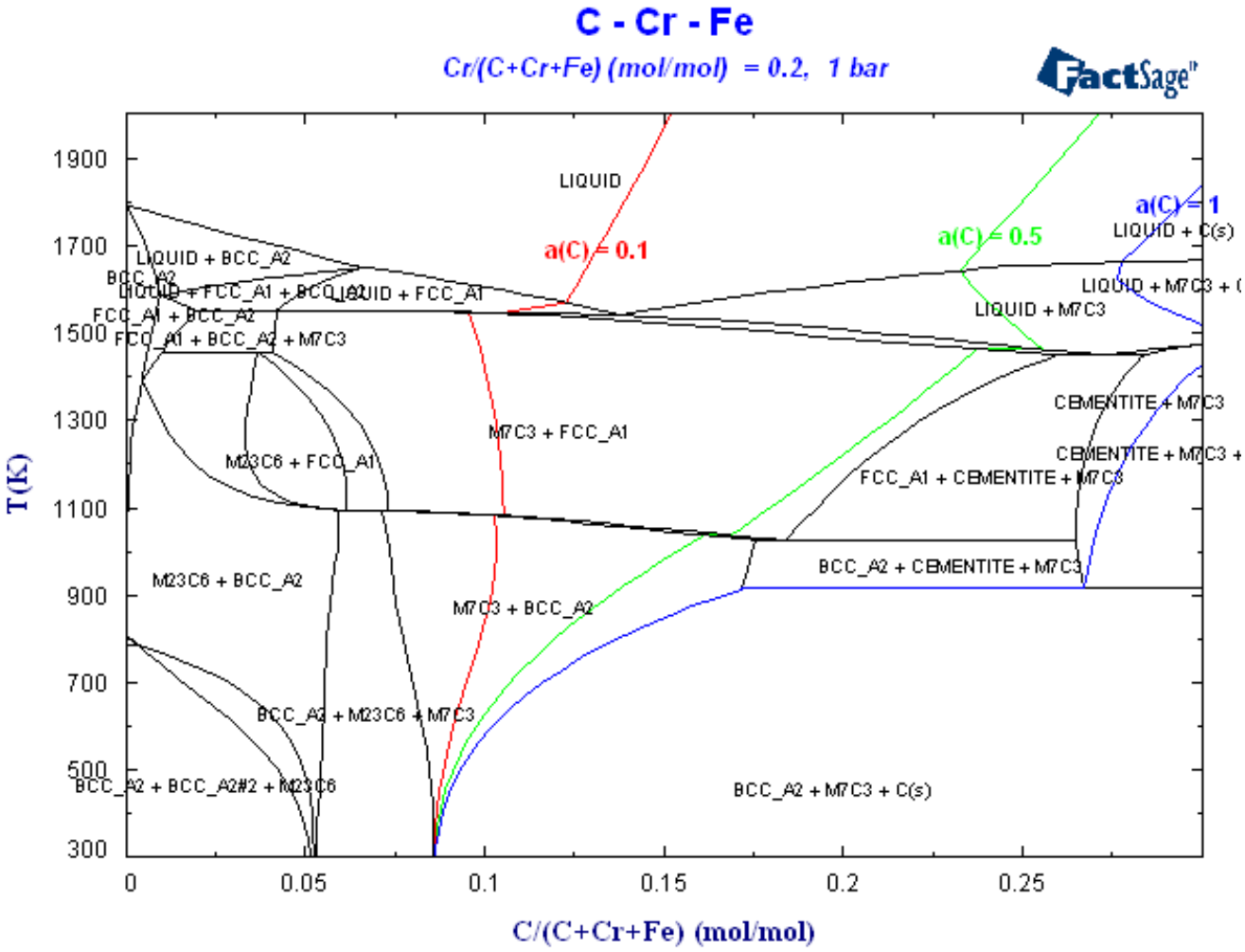
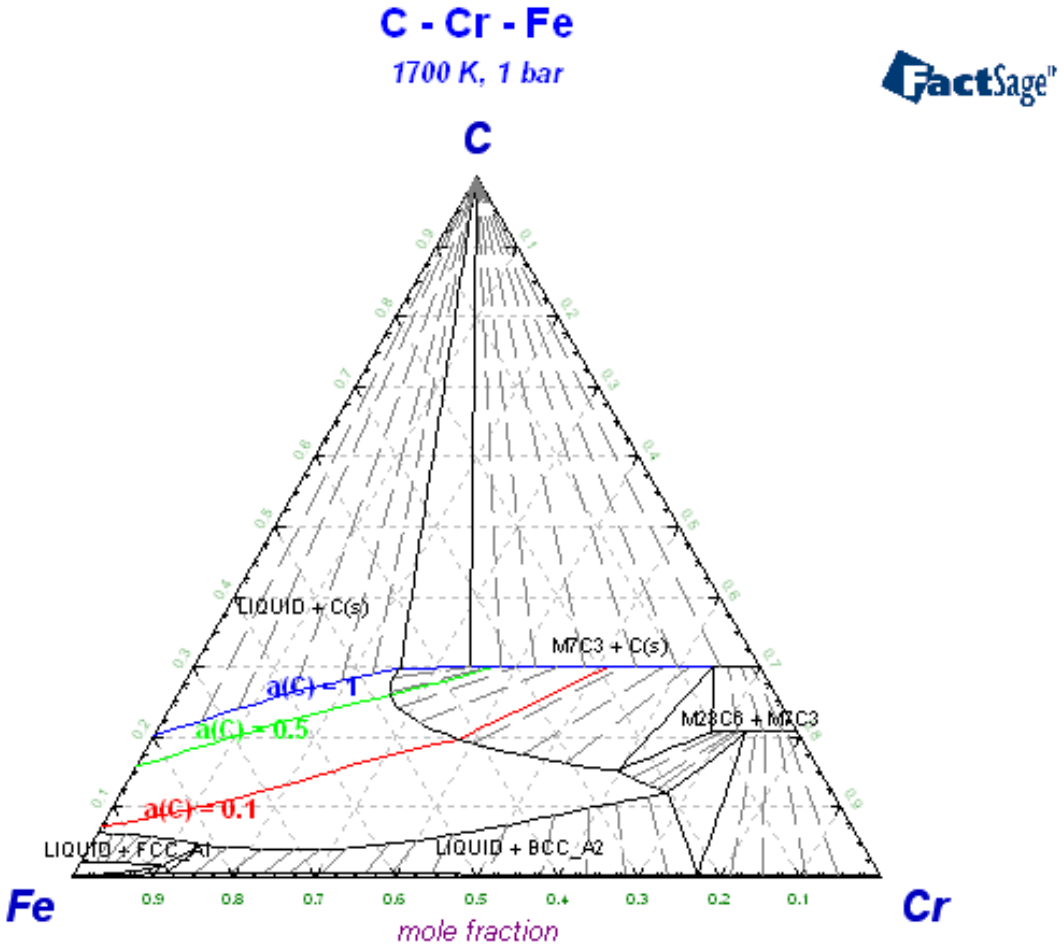
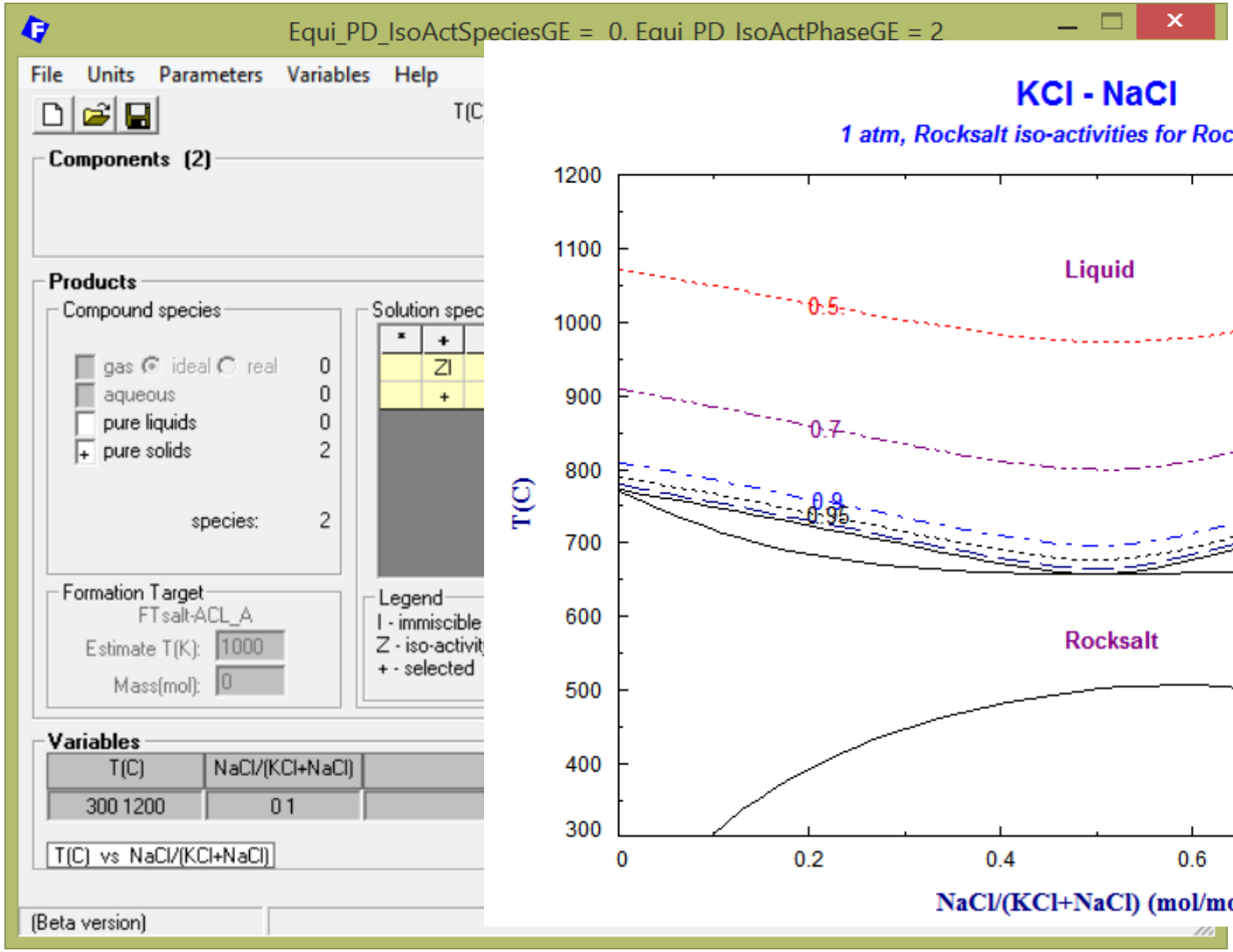

C - Cr - Fe
Cr/(C+Cr+Fe) (mol/mol) = 0.2, 1 bar
FactSage
LIQUID
a(C) = 0.1
a(C) = 0.5
a(C) = 1
LIQUID + C(s)
LIQUID + M7C3 + (
LIQUID + M7C3
LIQUID + BCC_A2
BCC_A2
LIQUID + FCC_A1 + BCC_A2
LIQUID + FCC_A1
FCC_A1 + BCC_A2
FCC_A1 + BCC_A2 + M7C3
CEMENTITE + M7C3
CEMENTITE + M7C3 +
FCC_A1 + CEMENTITE + M7C3
M7C3 + FCC_A1
M23C6 + FCC_A1
BCC_A2 + CEMENTITE + M7C3
M23C6 + BCC_A2
M7C3 + BCC_A2
BCC_A2 + M23C6 + M7C3
BCC_A2 + BCC_A2#2 + M23C6
BCC_A2 + M7C3 + C(s)
T(K)
1900
1700
1500
1300
1100
900
700
500
300
0
0.05
0.1
0.15
0.2
0.25
C/(C+Cr+Fe) (mol/mol)

… continued


C - Cr - Fe
1700 K, 1 bar
FactSage
C
LIQUID + C(s)
M7C3 + C(s)
a(C) = 1
a(C) = 0.5
a(C) = 0.1
M23C6 + M7C3
LIQUID + FCC_A1
LIQUID + BCC_A2
Fe
Cr
0.9 0.8 0.7 0.6 0.5 0.4 0.3 0.2 0.1
mole fraction

… continued


Equi_PD_IsoActSpeciesGE = 0, Equi_PD_IsoActPhaseGE = 2
File Units Parameters Variables Help
Components (2)
Products
Compound species
gas ideal real 0
aqueous 0
pure liquids 0
pure solids 2
species: 2
Solution spec
Formation Target
FTsalt-ACL_A
Estimate T(K): 1000
Mass(mol): 0
Legend
I - immiscible
Z - iso-activity
+ - selected
Variables
T(C)
NaCl/(KCl+NaCl)
300 1200
0 1
T(C) vs NaCl/(KCl+NaCl)
(Beta version)
C:\FactSage64\Figures\FS70\Rocksalt.IsoactivIties.bmp
29.06.2014
KCl - NaCl
1 atm, Rocksalt iso-activities for Rocksalt phase
FactSage
Liquid
Rocksalt
0.5
0.7
0.9
0.95
0.98
T(C)
NaCl/(KCl+NaCl) (mol/mol)
1200
1100
1000
900
800
700
600
500
400
300
0
0.2
0.4
0.6
0.8
1

There will be more to come !!!