

Processing - Combustion and Heat

1. Introduction to combustion
2. Compound databases : FactSage Browser & View Data - FACT53, SGPS
3. Simple combustion : $\text{CH}_4 + 2\text{O}_2 \Rightarrow \text{CO}_2 + 2\text{H}_2\text{O}$ – isothermal, adiabatic
4. Combustion in air : $\langle \text{Alpha} \rangle$ variable $\langle 1-A \rangle \text{CH}_4 + \langle 0.21A \rangle \text{O}_2 + \langle 0.79A \rangle \text{N}_2$
5. Real air and non-ideal calculations
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7. Equilibria : reduction kiln - pre-reduction of the Ni ore by ‘coke’ and ‘HSFO’
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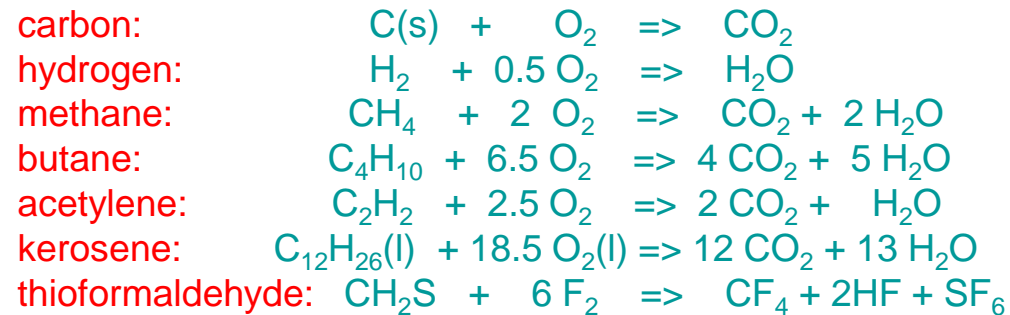
Introduction to combustion

Definition of combustion or burning:



Fuels often include organic compounds (especially hydrocarbons) in the gas, liquid or solid phase. Combustion reactions can be slow burning or rapid explosions

Many combustion reactions involve C-H-O where CO_2 and H_2O are the dominant product species.



None of the combustion reactions are stoichiometric as written above - product gases form complex chemical equilibria with O , O_3 , OH , H^+ , e^- etc. especially at high temperatures.



FactSage Browser - compound databases FACT53, SGPS

The image displays two overlapping screenshots of the FactSage Browser interface. The top screenshot shows the 'Summary of Databases' page, which lists various databases including FACT53 and SGPS. The bottom screenshot shows the detailed view for the FACT53 database, describing its contents and providing further information links.

FactSage 6.1 - Summary of Databases

Overview of databases

Compound Databases :

- FACT53** - FACT 5.3 compound database
- SGPS** - SGTE pure substances database

FACT53 - FACT general compound database

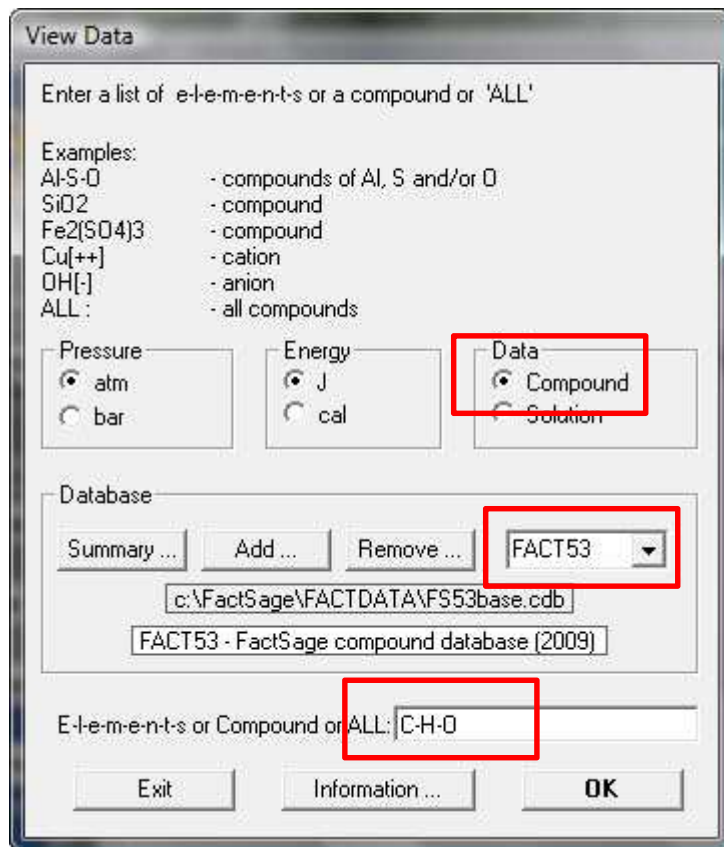
- contains data for over 4500 compounds (pure substances).
- contains data from standard compilations as well as most of the data for those compounds which have been evaluated / optimized to be thermodynamically consistent with the FACT FToxid, FTsalt, FThall, ... etc. solution databases (see below).
- **FACT53** database further information:
 1. **List of Compounds**,
 2. **Further Information**.

SGPS - SGTE pure substance database

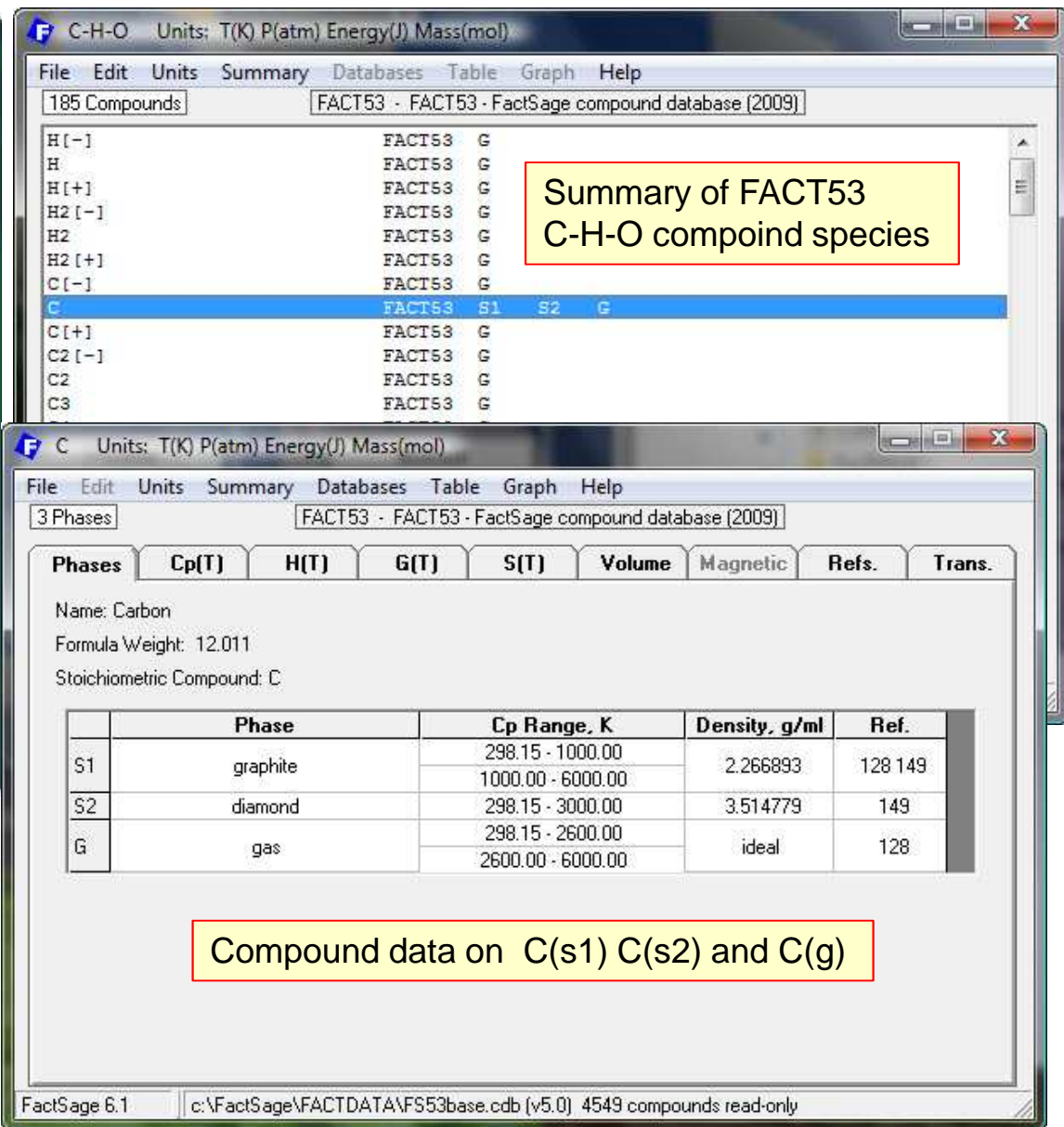
- contains data for for over 3400 compounds (pure substances) compiled by the SGTE groups.
- in general these data are not necessarily thermodynamically consistent with the SGTE solution databases.
- **SGPS** database further information:
 1. **List of Compounds**.

Revised: 06/06/2009

View Data - compound databases FACT53, SGPS



Compound Database : FACT53
 Elements : C-H-O



Reaction – Simple Combustion

Data Search

Databases - 1/24 compound databases, 0/22 solution databases

ELEM FSopp BINS
 FACT FSlead SGP
 Fact53 FSlite SGT
 FToxid FSstel SGN
 FTsalt FSupsi SGO
 FTmisc FSnobl SGN
 FThall TDm
 FThelg OLIP OLIG
 FTpulp OLIG OLIG
 FTlite OLIG OLIG

Information - Reaction only access
Click on a box to include (or exclude) a data compound and solution database (when available, note, this is NOT recommended).
If database is stored on your PC but not listed

Options
Default Include
 gaseous ion
 aqueous sp
 limited data

Cancel

Reactants - Reaction

File Edit Units Data Search Help

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

1 - 4

	Mass(mol)	Species	Phase	T(C)	P(atm)**	Activity	Data
	1	CH4	gas	25			
+	2	O2	gas	25			
=	1	CO2	gas	T			
+	2	H2O	gas steam	T			

non standard states

Next >>

FactSage 6.2 bet. Compound: 1/24 databases

Units: C, atm, J, mol
Data Search: Fact53
Phases: gas
Reactants: Standard states

Reaction – Simple Combustion

Table Reaction

File Units Output Figure Help

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

Reactants

CH₄ + 2 O₂ = CO₂ + 2 H₂O
(25C,g) (25C,g) (T,g) (T,g)

T(C)	Delta H(J)	Delta G(J)	Delta Vol(litre)	Delta S(J/K)	Delta Cp(J/K)	Delta A (J)	T
25.00	-802317.0	-800834.4	0.0000E+00	-4.973	9.924	-800834.4	
1000.00	-678227.8	-1479158.6	2.4002E+02	172.501	51.792	-1503478.5	
2000.00	-520300.2	-2296752.3	4.8619E+02	263.478	72.232	-2346015.8	
3000.00	-348655.9	-3189310.1	7.3237E+02	325.958	81.197	-3263517.1	
4000.00	-170464.8	-4136170.5	9.7854E+02	373.435	86.018	-4235321.0	
5000.00	11653.1	-5125576.4	1.2247E+03	411.718	89.342	-5249670.5	
5000.00	11653.1	-5125576.4	1.2247E+03	411.718	89.342	-5249670.5	T
4936.54	0.0	-5061684.7	1.2091E+03	409.495	89.141	-5184195.8	T

1. Set product T = 25 > calculate isothermal reaction
2. Set product T = 1000 - 5000 > calculate Delta(H) at T
3. Set Delta(H) = 11653.1 > calculate T = 5000 C
4. Set Delta(H) = 0 > adiabatic temperature 4936.54 C

0

Calculate << Back Clear

Equilib – Simple Combustion

Units: C, atm, J, mol

The screenshot shows the 'Reactants - Equilib' window in FactSage. The 'Units' menu is highlighted with a red box. Below it, a table lists the reactants:

Mass(mol)	Species	Phase	T(C)	P(total)**	Stream#	Data
1	CH4				1	
+ 2	O2				1	

Below the table, a yellow box contains the following text:

Reactants:
 $\text{CH}_4 + 2 \text{O}_2$
Initial conditions: not defined

An 'Initial Conditions' checkbox is located at the bottom right of the main area, also highlighted with a red box. A 'Next >>' button is at the bottom center. The status bar at the bottom shows 'FactSage 6.2 bet. Compound: 1/24 databases Solution: 0/22 databases'.

Equilib - Data Search

Reactants - Equilib

File Edit Table Units **Data Search** Help

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

1-2

Mass(mol)

1

+ 2

FactSage 6.2 bet. Comp...

Data Search

Databases - 2/24 compound databases, 0/22 solution databases

Fact **FactSage[®]** **SGTE**

ELEM FScomp BINS SGPS SGTE

FACT FSlead SGTE

Fact53 FSlite SGTE

FToxid FSstel SGnobl

FTsalt FSupsi SGsold

FTmisc FSnobl SGnucl

FTball TDnucl

FThelg **Other** OLIP OLIC

FTpulp OLIG OLIL

FTlite

compounds only

solutions only

no data

EXAM SGSL SGTE*

Clear All

Select All

Add/Remove Data

RefreshDatabases

Data Search:
Compound databases: **FACT53 & SGPS**
Options: **Default - no plasmas, C_xH_y, x=2**

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 (plasmas)

aqueous species

limited data compounds (25C)

Limits

Organic species C_xH_y... X(max) = 2

Minimum solution components: 1 2 cpts

Cancel Summary ... OK

Equilib Selection Window – simple combustion

Products -Compound species:
 Gases : FACT53 only (no duplicates)
 Liquids: none;
 Solids: C(s1) only

+	Code	Species	Data	Phase	T	V	Activity
+	33	C2H4O(g2)	FACT5	acetaldehyde			
+	34	CH3CH2OH(g)	FACT5	gas			
+	35	CH3CH2OH(g2)	FACT5	(ch3)2o			
+	36	HCOOH(g)	FACT5	gas			
+	37	CH3COOH(g)	FACT5	gas			
	38	H(g)	SGPS	g			
	39	H2(g)	SGPS	g			
	40	C(g)	SGPS	g			
	41	C2(g)	SGPS	g			
	42	C3(g)	SGPS	g			
	43	C4(g)	SGPS	g			
	44	C5(g)	SGPS	g			
	45	C60(g)	SGPS	g			
	46	CH(g)	SGPS	g			

Context Menu Options:
 Add all species containing: FACT53
 Add all species from database: SGPS
 Remove all species containing:
 Remove all species from database:

Equilib Menu Window – simple combustion

The screenshot shows the 'Equilib' menu window in FactSage 6.2 beta. The window title is 'Menu - Equilib: last system'. The menu includes 'File', 'Units', 'Parameters', and 'Help'. The units are set to T(C), P(atm), Energy(J), Mass(mol), and Vol(litre). The reactants are listed as 'CH4 + 2 O2'. The products section shows 'Compound species' with 'gas ideal' selected (37 species) and 'pure solids' selected (1 species), totaling 38 species. The 'Final Conditions' table is highlighted with a red box and contains the following data:

<A>		T(C)	P(atm)	Product H(J)
		0 5000 1000	1	

The 'Equilibrium' section is also highlighted with a red box and shows 'normal' selected. A yellow callout box contains the text: 'Final Conditions: Temperature; 0 5000 step 1000 Pressure: 1'. The 'Calculate >>' button is visible at the bottom right.

Equilib Results Window – FACT output

Results - Equilib 1000 C (page 2/5) FactSage 6.2 beta

Output Edit Show Pages

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

0 C -1000 C - 2000 C | 3000 C | 4000 C

CH4 + 2 O2 =

3.0000 mol gas_ideal
(80.040 gram, 3.0000 mol, 313.42 litre, 2.5538E-04 g/ml)
(1000.00 C, 1 atm, a=1.0000)

(0.66665	H2O	FACT53
+ 0.33332	CO2	FACT53
+ 1.1253E-05	H2	FACT53
+ 9.7979E-06	O2	FACT53
+ 9.1820E-06	CO	FACT53
+ 1.6802E-06	OH	FACT53
+ 2.3840E-09	H	FACT53
+ 3.3559E-10	O	FACT53
+ 1.1425E-10	HOO	FACT53

The cutoff concentration has been specified to 1.0000E-10

H	G	V	S	Cp
(J)	(J)	(litre)	(J/K)	(J/K)
-7.53084E+05	-1.75201E+06	3.13419E+02	7.84609E+02	1.46408E+02

Total mass/gram = 80.040

T = 1000.00 C
P = 1.00000E+00 atm

Results:
FACT vs ChemSage Output
Print cut-off 10⁻¹⁰

Equilib Results Window – Chemsage output

Results - Equilib 1000 C (page 2/6) FactSage 6.2 beta

Output Edit Show Pages

Save or Print ▶ T(C) P(atm) Energy(J) Mass(mol) Vol(litre)

Plot ▶ 4000 C | 5000 C |

Equilib Results file ▶ has been specified to 1.0000E-10

Stream File ▶

Format ▶

Fact-XML ▶

Fact-Optimal ▶

Refresh ...

FACT Format Cp (J/K)

ChemSage Format

✓ FACT + ChemSage

ChemSage + FACT

2 1.46408E+02

~~~~~

T = 1000.00 C  
P = 1.00000E+00 atm  
V = 3.13419E+02 dm3

STREAM CONSTITUENTS AMOUNT/mol

|     |            |
|-----|------------|
| CH4 | 1.0000E+00 |
| O2  | 2.0000E+00 |

PHASE: gas\_ideal

|     | EQUIL AMOUNT mol | MOLE FRACTION | FUGACITY atm |
|-----|------------------|---------------|--------------|
| H2O | 2.0000E+00       | 6.6665E-01    | 6.6665E-01   |
| CO2 | 9.9997E-01       | 3.3332E-01    | 3.3332E-01   |
| H2  | 3.3760E-05       | 1.1253E-05    | 1.1253E-05   |
| O2  | 2.9394E-05       | 9.7979E-06    | 9.7979E-06   |
| CO  | 2.7546E-05       | 9.1820E-06    | 9.1820E-06   |
| OH  | 5.0407E-06       | 1.6802E-06    | 1.6802E-06   |
| H   | 7.1520E-09       | 2.3840E-09    | 2.3840E-09   |
| O   | 1.0068E-09       | 3.3559E-10    | 3.3559E-10   |

Results:  
ChemSage Output

# Equilib – Duplicate data in Fact53 & SGPS

Menu - Equilib: last system

File Units Parameters Help

T(C) P(atm) Energy(J)

Reactants (2)

CH4 +

Products

Compound species

- gas  ideal  real 45
- aqueous 0
- pure liquids 0
- pure solids 4

suppress duplicates apply

species: 49

suppress duplicates > apply

Selection - Equilib

File Edit Show Sort

Selected: 45/84 Duplicates selected. GAS Sorted by Code

| + Code | Species      | Data   | Phase   | T | V | Activity |
|--------|--------------|--------|---------|---|---|----------|
| 34     | CH3CH2OH(g)  | FACT53 | gas     |   |   |          |
| 35     | CH3CH2OH(g2) | FACT53 | (ch3)2o |   |   |          |
| 36     | HCOOH(g)     | FACT53 | gas     |   |   |          |
| 37     | CH3COOH(g)   | FACT53 | gas     |   |   |          |
| 38     | H(g)         | SGPS   | g       |   |   |          |
| 39     | H2(g)        | SGPS   | g       |   |   |          |
| 40     | C(g)         | SGPS   | g       |   |   |          |
| 41     | C2(g)        | SGPS   | g       |   |   |          |
| 42     | C3(g)        | SGPS   | g       |   |   |          |
| 43     | C4(g)        | SGPS   | g       |   |   |          |
| 44     | C5(g)        | SGPS   | g       |   |   |          |
| 45     | C60(g)       | SGPS   | g       |   |   |          |
| 46     | CH(g)        | SGPS   | g       |   |   |          |
| 47     | CH2(g)       | SGPS   | g       |   |   |          |

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

Final Conditions

|     |     |             |        |              |
|-----|-----|-------------|--------|--------------|
| <A> | <B> | T(C)        | P(atm) | Product H(J) |
|     |     | 0 5000 1000 | 1      |              |

10 steps  Table 6 calculations

Equilibrium

- normal  normal + transitions
- transitions only  open
- predominant

Calculate >>

FactSage 6.2 beta

# Equilib Reactants Window – combustion in air

Data Search: FACT53 only

Reactants - Equilib

File Edit Table Units Data Search Help

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

1 - 3

| Mass(mol) | Species | Phase | T(C) | P(total)** | Stream# | Data |
|-----------|---------|-------|------|------------|---------|------|
| <1-A>     | CH4     | gas   | 25   | 1          | 1       |      |
| + <0.21A> | O2      | gas   | 25   | 1          | 1       |      |
| + <0.79A> | N2      | gas   | 25   | 1          | 1       |      |

**Reactants:**  
<1-A> CH<sub>4</sub> + <0.21A> O<sub>2</sub> + <0.79A> N<sub>2</sub>  
Initial conditions: defined

\*\*\* P(total) is the hydrostatic pressure above the phase.  
For a gaseous stream this is the sum of the partial pressures of the species in that stream.

Initial Conditions

Next >>

FactSage 6.2 bet. Compound: 1/24 databases Solution: 0/22 databases

# Equilib Menu Window – combustion in air

The screenshot shows the 'Equilib' menu window in FactSage 6.2 beta. The window title is 'Menu - Equilib: last system'. The menu includes 'File', 'Units', 'Parameters', and 'Help'. The units are set to T(C), P(atm), Energy(J), Mass(mol), and Vol(litre). The reactants are listed as <1-A> CH4, <0.21A> O2, and <0.79A> N2, all at 25C,g,#1. The products section is currently empty. The 'Final Conditions' section shows a table with columns for <A>, <B>, T(C), P(atm), and Delta H(J). The table contains the values 0, 1, 0.01, 1, and 0. The 'Equilibrium' section is set to 'normal'. The 'Calculate >>' button is visible.

**Reactants (3)**

<1-A> CH4 + <0.21A> O2 + <0.79A> N2  
(25C,g,#1) (25C,g,#1) (25C,g,#1)

**Products**

Compound species: gas (ideal) 73, aqueous 0, pure liquids 0, pure solids 1. suppress duplicates apply. custom selection species: none.

**Final Conditions**

| <A> | <B> | T(C) | P(atm) | Delta H(J) |
|-----|-----|------|--------|------------|
| 0   | 1   | 0.01 | 1      | 0          |

10 steps, 101 calculations

**Equilibrium**

normal (selected), normal + transitions, transitions only, predominant. Calculate >>

**Final Conditions:**  
<A>: 0 1 step 0.01  
Temperature: undefined  
Pressure: 1  
Delta(H): 0

# Equilib Results Window – combustion in air

The screenshot shows the 'Equilib Results' window in FactSage 6.2 beta. The window title is 'Results - Equilib 1956.74 C, A=0.9 (page 91/101) FactSage 6.2 beta'. The 'Output' menu is open, highlighting 'Plot Results ...'. The main window displays a table of species and their properties, including temperature (T), pressure (P), energy (Energy), mass (Mass), and volume (Vol).

|  | T(C)              | P(atm)            | Energy(J)         | Mass(mol)         | Vol(litre)        |
|--|-------------------|-------------------|-------------------|-------------------|-------------------|
|  | 1409.81 C, A=0.84 | 1500.55 C, A=0.85 | 1593.1 C, A=0.86  |                   |                   |
|  | 6 C, A=0.78       | 979.48 C, A=0.79  | 1062.76 C, A=0.8  |                   |                   |
|  | 0.94              | 1207.27 C, A=0.95 | 999.2 C, A=0.96   | 779.19 C, A=0.97  | 545.05 C, A=0.98  |
|  | 88                | 1880.48 C, A=0.89 | -1956.74 C, A=0.9 | 1907.28 C, A=0.91 | 1763.51 C, A=0.92 |

Species list:

- + <0.79A> N2 = (25, 1, g, #1)
- deal
- mol, 185.55 litre, 1.4858E-04 g/ml)
- (1956.74 C, 1 atm, a=1.0000)
- ( 0.70068 N2
- + 0.18804 H2O
- + 8.0820E-02 CO2
- + 1.7796E-02 CO
- + 7.8546E-03 H2
- + 2.0908E-03 OH
- + 1.0689E-03 O2
- + 9.5892E-04 NO
- + 5.8675E-04 H
- + 1.0593E-04 O
- + 3.0315E-07 HOO
- + 7.7384E-08 NO2
- + 4.5343E-08 N2O
- + 3.5895E-08 HNO
- + 2.2710E-08 HOOH
- + 1.4721E-08 N
- + 8.6693E-09 NH3
- + 3.2471E-09 HONO (g2)
- + 2.8037E-09 HONO (g)

Output >  
Plot Results ...



# Equilib Results Window - combustion in air - plot results

The image shows the 'Equilib Results Window' in FactSage 6.1. The main window displays a table of results and a list of variables. The 'Axes' list is open, showing the following variables:

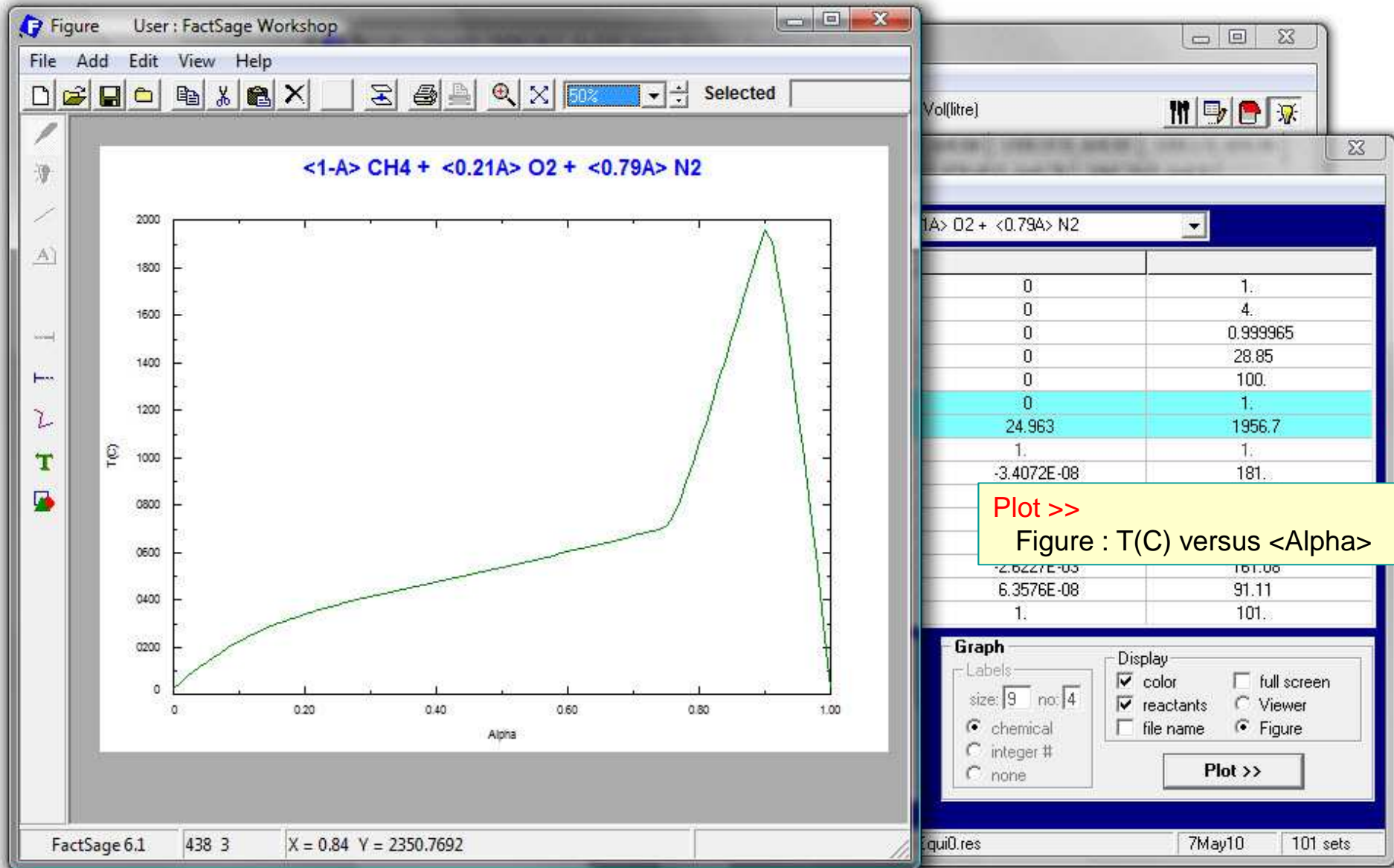
- activity
- mole
- mole fract.
- gram
- weight %
- Alpha
- T(C)
- P(atm)
- Delta Cp(J)
- Delta G(J)
- Vol(litre)
- Delta H(J)
- Delta V(litr)
- Delta S(J)
- page -
- Y
- log10(Y)
- ln(Y)
- exp(Y)
- 1/Y
- phase distribution

The 'Axes: T(C) vs Alpha' dialog box is open, showing the following settings:

- Y-axis: T(C)
- X-axis: Alpha
- Y-axis maximum: 2000
- Y-axis minimum: 0
- Y-axis tick every: 100
- X-axis maximum: 1
- X-axis minimum: 0
- X-axis tick every: 0.1

The dialog box also has 'Cancel', 'Refresh', and 'OK' buttons. A yellow callout box points to the 'Axes > T(C) versus <Alpha> ...' option in the main window's 'Axes' list.

# Equilib Results Window - combustion in air - plot results



# Equilib Results Window - export results to Excel

The screenshot shows the 'Equilib Results Window' in FactSage 6.2 beta. The window title is 'Results - Equilib 1956.74 C, A=0.9 (page 91/101) FactSage 6.2 beta'. The 'Output' menu is open, showing options like 'Save or Print', 'Plot', 'Equilib Results file', 'Stream File', 'Format', 'Fact-XML', 'Fact-Optimal', and 'Refresh ...'. A yellow callout box points to the 'Output' menu with the text 'Output> Export to Excel file etc.'. Below the menu, a table of results is visible, showing mass and volume for various species at different temperatures and air-fuel ratios.

| Species   | Mass (mol) | Volume (litre) |
|-----------|------------|----------------|
| N2        | 0.70068    |                |
| H2O       | 0.18804    |                |
| CO2       | 8.0820E-02 |                |
| CO        | 1.7796E-02 |                |
| H2        | 7.8546E-03 |                |
| OH        | 2.0908E-03 |                |
| O2        | 1.0689E-03 |                |
| NO        | 9.5892E-04 |                |
| H         | 5.8675E-04 |                |
| O         | 1.0593E-04 |                |
| HOO       | 3.0315E-07 |                |
| NO2       | 7.7384E-08 |                |
| N2O       | 4.5343E-08 |                |
| HNO       | 3.5895E-08 |                |
| HOOH      | 2.2710E-08 |                |
| N         | 1.4721E-08 |                |
| NH3       | 8.6693E-09 |                |
| HONO (g2) | 3.2471E-09 |                |
| HONO (g)  | 2.8037E-09 |                |

The 'Output' dialog box is open, showing the 'Page Range' section with 'All 101 pages' selected and 'Current page 91' unselected. The 'Type of Output' section has 'Excel Spreadsheet' selected, with 'Spreadsheet setup ...' button next to it. Other options include 'Printer', 'Text file (\*.txt)', 'Equilib Results File (Equi\*.res)', and 'Xml file (\*.xml)'. The 'OK' button is highlighted.

# Mixtures – Mixture Module



# Mixtures – real air

The screenshot shows the FactSage 'Mixtures and Streams' window. The main table lists the components of the mixture:

| Mass(mol) | Species | Phase | T(C) | P(total) |
|-----------|---------|-------|------|----------|
| 0.78084   | N2      | gas   | 25   | 1        |
| + 0.20946 | O2      | gas   | 25   | 1        |
| + 0.00939 | Ar      | gas   | 25   | 1        |
| + 0.00031 | CO2     | gas   | 25   | 1        |

A yellow callout box on the left states: **Real air: 1 mole gas mixture at 25°C:**  
 $0.78084 \text{ N}_2 + 0.20946 \text{ O}_2 + 0.00939 \text{ Ar} + 0.00031 \text{ CO}_2$

A yellow callout box on the right says: **Save mixture in [Air\_Real]**

A 'Save File' dialog box is open, showing the file name 'Air\_Real' entered in the text field. The dialog prompts for a stream file number or name and lists special characters to avoid.

At the bottom left of the main window, a red box highlights the 'total moles' field, which contains the value '1'.

The status bar at the bottom of the window shows: FactSage 6.2 bet. Compound: 1/24 databases c:\Workshop\Processing\MixAir\_Real.DAT

# Mixtures – real air

The screenshot shows two windows from the FactSage software. The background window is titled 'Mixtures and Streams' and has a menu open with 'File > Directories ...' selected. The foreground window is titled 'Directory Mixtures and Streams - file c:\Workshop\Processing\MixtAir\_Real.DAT' and displays a table of files.

**File > Directories ....**  
Directory of Mixtures

| File       | Date   | Description                                                                                |
|------------|--------|--------------------------------------------------------------------------------------------|
| Air_Real   | 2May10 | Combustion calculations mixture / 0.78084 N2 + 0.20946 O2 + 0.00939 Ar + 0.00031 CO2       |
| Air_Simple | 2May10 | Combustion calculations mixture / 0.79 N2 + 0.21 O2                                        |
| Ni_ore     | 4May10 | Ni feed for reduction kiln mixture / 21 MgO + 45.228 SiO2 + 31 Fe2O3 + 2.672 NiO + 0.1 CoO |

# Mixtures – importing [Air\_Real] mixture into Equilib

The top screenshot shows the 'Reactants - Equilib' window with the 'File' menu open. The 'Mixtures and Streams' option is selected, and the 'Import a mixture' sub-menu is open, showing the following options:

- Import a mixture
- Import a stream (or single-line mixture)
- Edit a mixture or stream
- Directory (c:\FactWin\Processing\)

The bottom screenshot shows the 'Reactants - Equilib' window with a table of reactants. The table has the following columns: Mass(mol), Species, Phase, T(C), P(total)\*\*, and Stream#. The table contains two rows:

| Mass(mol) | Species    | Phase    | T(C)    | P(total)** | Stream# | Data |
|-----------|------------|----------|---------|------------|---------|------|
| <1-A>     | CH4        | gas      | 1000.00 | 1.0        | 1       |      |
| + <A>     | [Air_Real] | [Stream] | 25      | 1          | 2       |      |

The dropdown menu for the '[Air\_Real]' mixture is open, showing the following options:

- [Air\_Real]
- Combustion\_calculation
- Mole fractions:
- 1.0000E+00 Total
- 7.8084E-01 N2
- 2.0946E-01 O2
- 9.3900E-03 Ar
- 3.1000E-04 CO2

# Equilib – Data Search options

**Options**

Default

**Include**

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

**Limits**

Organic species CxHy..., X(max) = 4

Minimum solution components:  1  2 cpts

Reactants - Equilib

File Edit Table Units **Data Search** Help

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

1-2

| Mass(mol) | Species    | Phase    | T(C) | P(total)** | Stream# | Data |
|-----------|------------|----------|------|------------|---------|------|
| <1-A>     | CH4        | gas      | 25   | 1.0        | 1       |      |
| + <A>     | [Air_Real] | [Stream] | 25   | 1          | 2       |      |

**Data Search > Options :**

- include gaseous ions (plasmas)
- up to 4 carbon atoms per molecule

Initial Conditions

Next >>

FactSage 6.2 bet. Compound: 1/24 databases Solution: 0/22 databases



# Equilib Menu Window – real gas adiabatic settings

The screenshot shows the 'Equilib' menu window in FactSage 6.2 beta. The window title is 'Menu - Equilib: last system'. The menu bar includes 'File', 'Units', 'Parameters', and 'Help'. The main area is divided into several sections:

- Reactants (2):** <1-A> CH<sub>4</sub> (25C,g,#1) + <A> [Air\_Real] (25C,#2)
- Products:**
  - Compound species:**  gas  ideal  real 152;  aqueous 0
  - pure liquids 0
  - pure solids 1
  - suppress duplicates apply
  - \* custom selection species: 153
- Target:** Estimate T(C): 1000; Mass(mol): 0
- Legend:**  Show  all  selected; species: 0; solutions: 0; Select
- Custom Solutions:**  fixed activities;  ideal solutions;  activity coefficients; Details ...
- Pseudonyms:** apply  List ...
- include molar volumes
- Total Species (max 1500) 153
- Total Solutions (max 40) 0
- Default

**Final Conditions:** A table with columns <A>, <B>, T(C), P(atm), and Delta H(J). The <A> column contains '0.90', T(C) is empty, P(atm) is '1', and Delta H(J) is '0'. Below the table are '10 steps' and 'Table' checkboxes.

**Equilibrium:**  normal  normal + transitions;  transitions only  open;  predominant; Calculate >>

A yellow text box in the center of the window reads: 'Real gas adiabatic calculation with <A> = 0.90'. Red boxes highlight the 'real' radio button in the compound species section, the '0.90' value in the final conditions table, the 'T(C)' column header, and the '0' value in the Delta H(J) column.

# Equilib Results Window – real gas adiabatic temperature

Results - Equilib 1956.59 C FactSage 6.2 beta

Output Edit Show Pages

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

```

<1-A> CH4 + <A> [Air_Real] =
(25,1,g,#1) (25,1,stream,#2)

1.0144 mol gas_real
(27.673 gram, 1.0144 mol, 185.61 litre, 1.4910E-04
(1956.59 C, 1 atm, a=1.0000)
  
```

Double-Click on H2O for View Data

Gaseous ions (plasma)

<A> = 0.90, Delta(H) = 0  
=> Product T = 1956.59 °C

H2O Units: T(C) P(atm) Energy(J) Mass(mol)

File Edit Units Summary Databases Table Graph Help

3 Phases FACT53 - FACT53 - FactSage compound database (2009)

Phases Cp(T) H(T) G(T) S(T) Volume Magnetic Refs. Trans.

Name: Water  
Volume data

Non-ideal gas properties

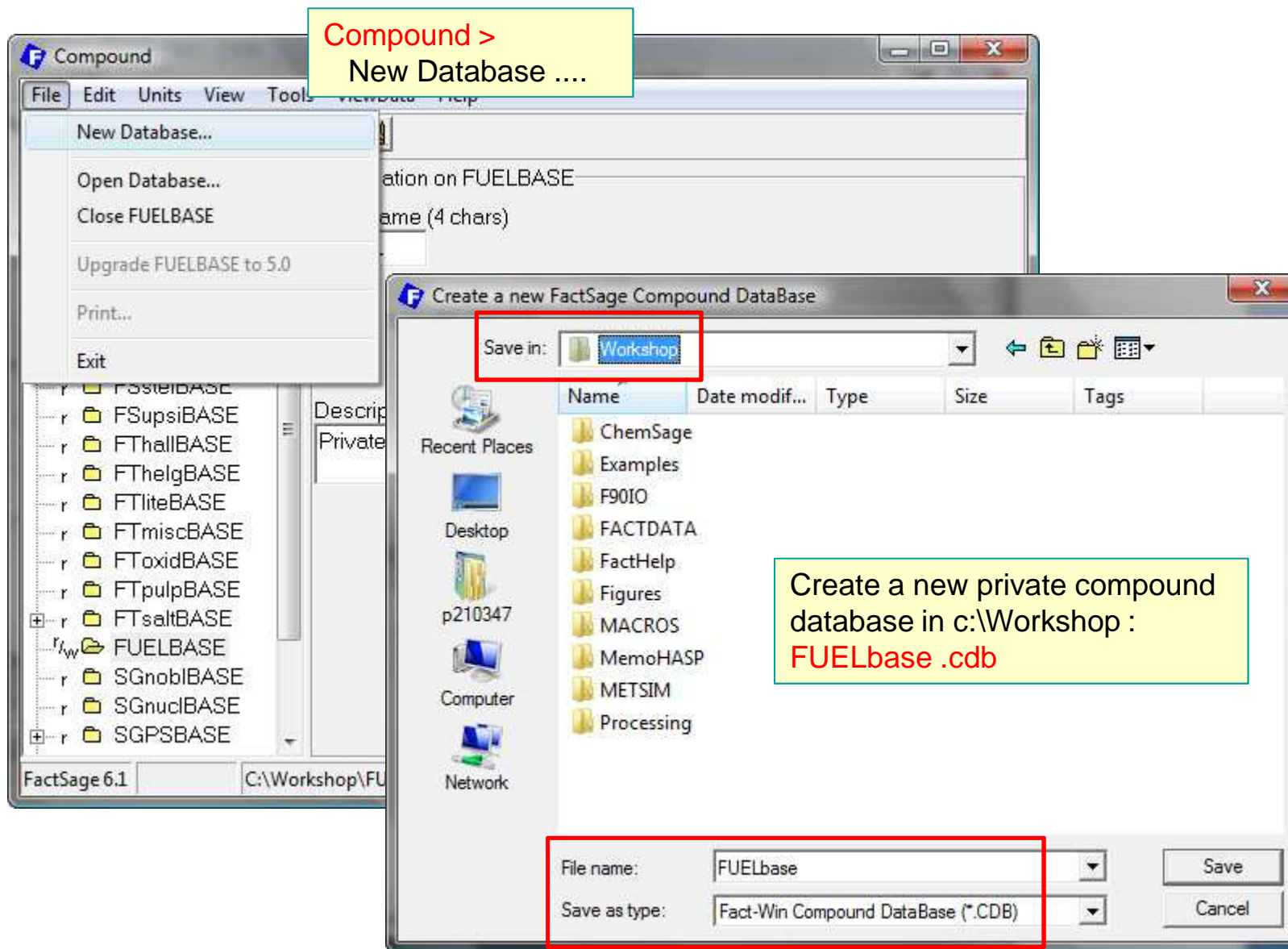
|   | Tc      | Pc      | Vc       | Omega | Dipole Moment |
|---|---------|---------|----------|-------|---------------|
|   | (K)     | (bar)   | (cc/mol) |       | (Debyes)      |
| G | 647.300 | 221.200 | 57.100   | 0.344 | 1.800         |

Expansivities / Compressibilities / Derivative of Bulk  
(-none-)

View Data  
- non-ideal gas properties of H<sub>2</sub>O(g)

FactSage 6.1 c:\FactSage\FACTDATA\FS53base.cdb (v5.0) 4549 compounds read-only

# Compound – new private database



# Compound – new private fuel data on 'coke'

Energy: Joules Pressure: atm C

File Edit Units View Tools ViewData Help

Formula: C

BINSBASE  
ELEMBASE  
FACT53BASE  
C  
FACTBASE  
FScoppBASE  
FSleadBASE  
FSliteBASE  
FSnoblBASE  
FSstelBASE  
FSupsiBASE  
FThallBASE  
FThelgBASE  
FTliteBASE  
FTmiscBASE  
FToxidBASE  
FTpulpBASE  
FTsaltBASE  
FUELBASE  
C  
S1  
SGnoblBASE

C properties  
Weight: 12.011 g/mol Modified: 2010 May 07  
Compound Name Reference no.  
coke 128 149  
Comments  
private compound data on 'coal'

Drag and drop C(s1) from FACT53  
Save 'coke' in FUELbase.cdb

FactSage 6.1 Modified C:\Workshop\FUELBASE.CDB (v5.0) 1 compounds read/write

# Compound – new private fuel data on ‘anthracite’ & ‘HSFO’

**Fuel #2:**

- Gross heating - H<sub>2</sub>O(l) product
- Heat = 14000 btu/lb
- Weight %90% C + 10 %H
- save as solid 'anthracite'

**Fuel #3:**

- Net heating - H<sub>2</sub>O(l) product
- Net heat = 18300 btu/lb
- Weight% 87% C, 9.8 %H, 3.2%S
- Save as liquid 'HSFO'
- high sulfur fuel oil

**Fuel Properties (Fuel #3):**

Formula: SC73H97  
DH form: -130027.429234512 J/mol  
DH form: -55.7866644547237 BTU/lb  
Weight: 1002.0625 g/mol  
Cp: 2004 J/mol.K

# View Data – summary of FUEL compound data

The 'View Data' dialog box is shown on the left. It contains the following elements:

- Input field: "Enter a list of e-l-e-m-e-n-t-s or a compound or 'ALL'"
- Examples list:
  - Al-S-O: - compounds of Al, S and/or O
  - SiO2: - compound
  - Fe2(SO4)3: - compound
  - Cu[++] : - cation
  - OH[-] : - anion
  - ALL : - all compounds
- Pressure: atm (selected), bar
- Energy: J (selected), cal
- Data: Compound (selected), Solution
- Database: Summary..., Add..., Remove..., FUEL (dropdown), C:\Workshop\FUELBASE.CDB, Private Fuel compound database
- Input field: "E-l-e-m-e-n-t-s or Compound or ALL: ALL"
- Buttons: Exit, Information..., OK

The 'ALL compounds' window is shown on the right. It displays the following data:

| FUEL - Private Fuel compound database |      |    |    |   |
|---------------------------------------|------|----|----|---|
|                                       | FUEL | S1 | S2 | G |
| C                                     | FUEL | S1 | S2 | G |
| CH                                    | FUEL | S  |    |   |
| SC73H97                               | FUEL | L  |    |   |

FactSage 6.1 | C:\Workshop\FUELBASE.CDB (v5.0) 3 compounds read/write

# Equilib – combustion of HSFO ‘high sulfur fuel oil’

The screenshot displays the FactSage software interface for an equilibrium calculation. The main window, titled "Reactants - Equilib", shows a table of reactants:

| Mass(lb) | Species | Phase            |
|----------|---------|------------------|
| 1        | SC73H97 | liquid-FUEL hsfo |
| + 6      | O2      | gas-FACT53       |

The "Data Search" dialog box is open, showing a list of databases. The "Fact53" and "FUEL" databases are selected (checked). The "Miscellaneous" section also shows "EXAM" and "SGTE\*" as options. A yellow box highlights the text "Fact53 and FUEL compound databases".

At the bottom of the "Reactants - Equilib" window, the status bar shows "FactSage 6.2 beta", "Compound: 2/25 databases", and "Solution: 0/22 databases".

# Equilib – combustion of HSFO ‘high sulfur fuel oil’

**Menu - Equilib: last system**

File Units Parameters Help

T(F) P(psi) Energy(Btu) Mass(lb) Vol(ft3)

**Reactants (2)**

(lb) SC73H97 + 6 O2  
(77F\_liq-FUEL,#1) (77F\_g-FACT53,#1)

**Products**

Compound species  
 gas  ideal  real 64  
 aqueous 0  
 pure liquids 1  
 pure solids 0  
 suppress duplicates apply  
\* - custom selection  
species: 65

Solution species  
- none -

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

Legend  
 Show  all  selected  
species: 0  
solutions: 0

**Final Conditions**

| <A> | <B> | T(F) | P(psi) | Delta H(Btu) |
|-----|-----|------|--------|--------------|
|     |     | 77   | 14.7   |              |

10 steps  Table 1 calculation

FactSage 6.2 beta c:\Workshop\Processing\EquiCombustion\Anthracite.DAT

**Results - Equilib 77 F FactSage 6.2 beta**

Output Edit Show Pages

T(F) P(psi) Energy(Btu) Mass(lb) Vol(ft3)

(lb) SC73H97 + 6 O2 =  
(77,1,liq-FUEL,#1) (77,1,g-FACT53,#1)

76.241 mol gas\_ideal  
(2828.8 gram, 76.241 mol, 1864.8 litre, 1.5170E-03 g/ml)  
(77.00 F, 14.700 psi, a=1.0000)  
( 0.53376 O2  
+ 0.42898 CO2  
+ 3.1344E-02 H2O  
+ 5.9102E-03 O2S(OH)2

+ 0.75901 lb H2O\_liquid  
(344.28 gram, 19.110 mol)  
(77.00 F, 14.700 psi, L1, a=1.0000)

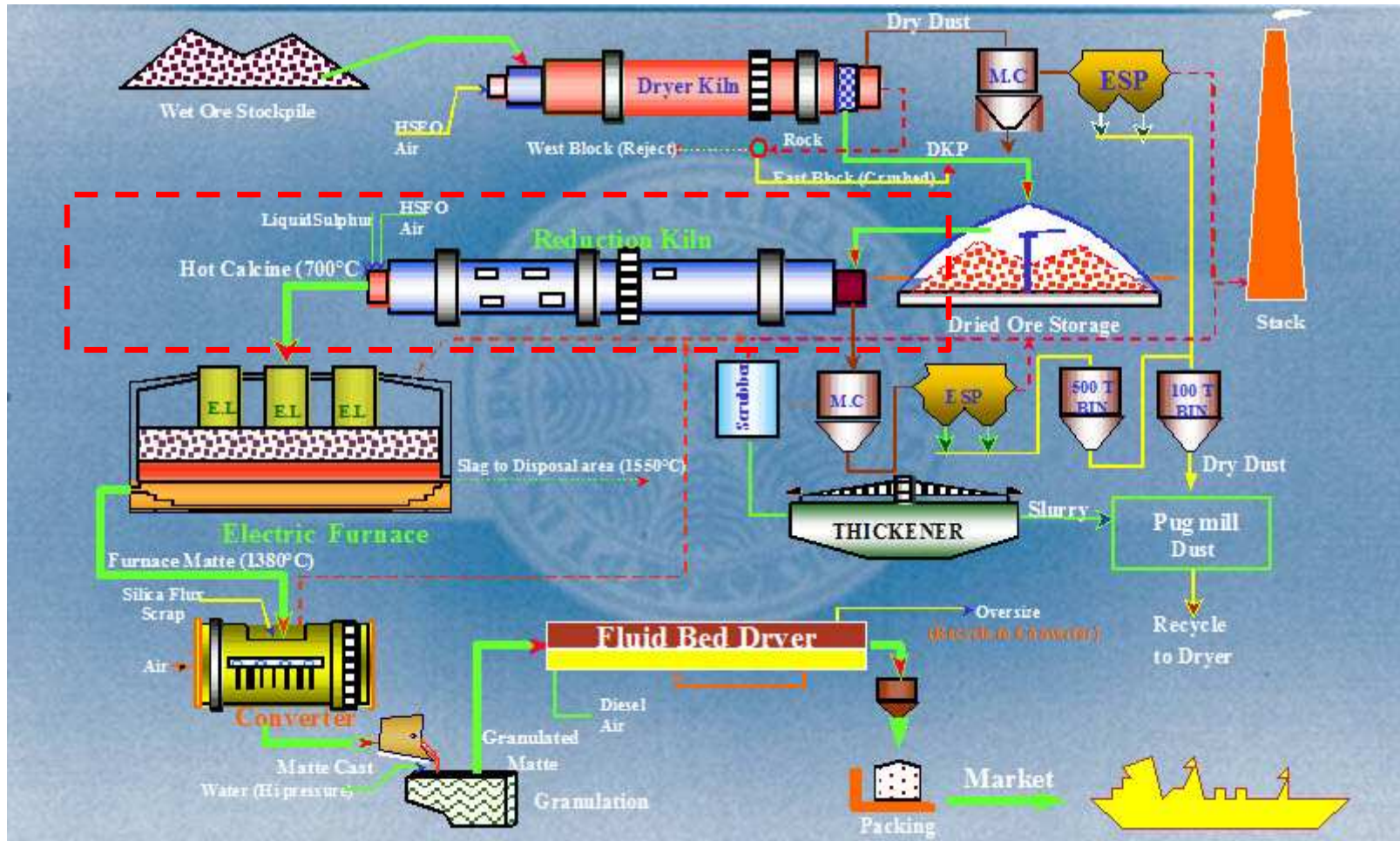
The cutoff concentration has been specified to 1.0000E-10

| DELTA H<br>(Btu) | DELTA G<br>(Btu) | DELTA V<br>(ft3) | DELTA S<br>(Btu/F) | DELTA C<br>(Btu/F) |
|------------------|------------------|------------------|--------------------|--------------------|
| -1.81823E+04     | -1.77442E+04     | -1.01407E+03     | -8.16334E-01       | 3.70051E           |

**Net heat of combustion**



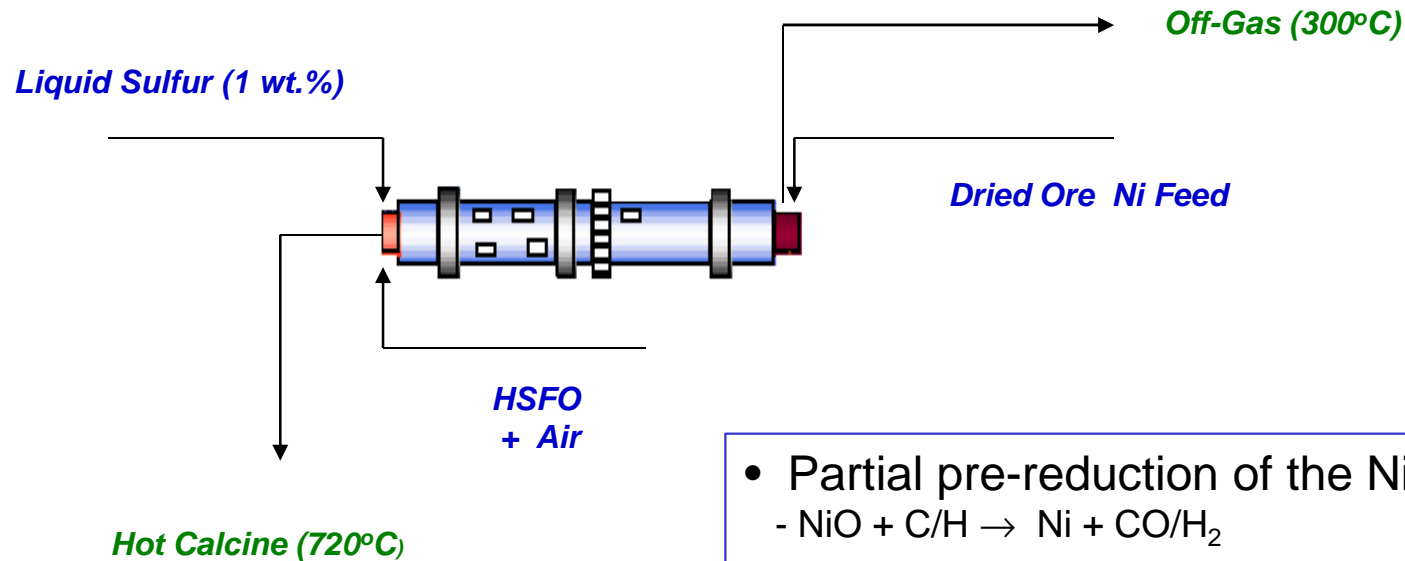
# Databases – Reduction Kiln



## Databases

|               |                                          |
|---------------|------------------------------------------|
| <b>FUEL</b>   | HSFO, coke                               |
| <b>Fact53</b> | Liquid Sulfur, Off-Gas                   |
| <b>FTOxid</b> | Hot Calcine (O-products), Dried Ore Feed |
| <b>FTMisc</b> | Hot Calcine (S-products)                 |

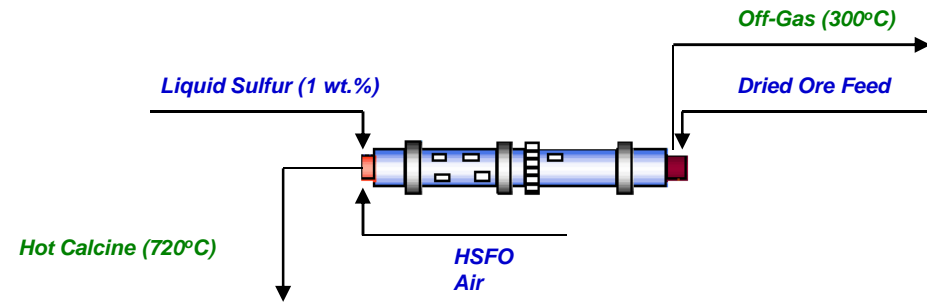
## Reduction Kiln



- Partial pre-reduction of the Ni ore
  - $\text{NiO} + \text{C/H} \rightarrow \text{Ni} + \text{CO/H}_2$
- Sulfuration of the Ni
  - $\text{NiO} + \text{C/H} + \text{S} \rightarrow \text{Ni}_3\text{S}_2 + \text{CO/H}_2$
- Preheat the mineral
  - combustion of high sulfur fuel oil 'HSFO'  $\Rightarrow 720^\circ\text{C}$
  - not too hot - must avoid liquid phases and calcine sinter
- Remove last traces of water

# Equilib – Reduction kiln

Products at 720°C : Pre-reduction of Ni & Fe;



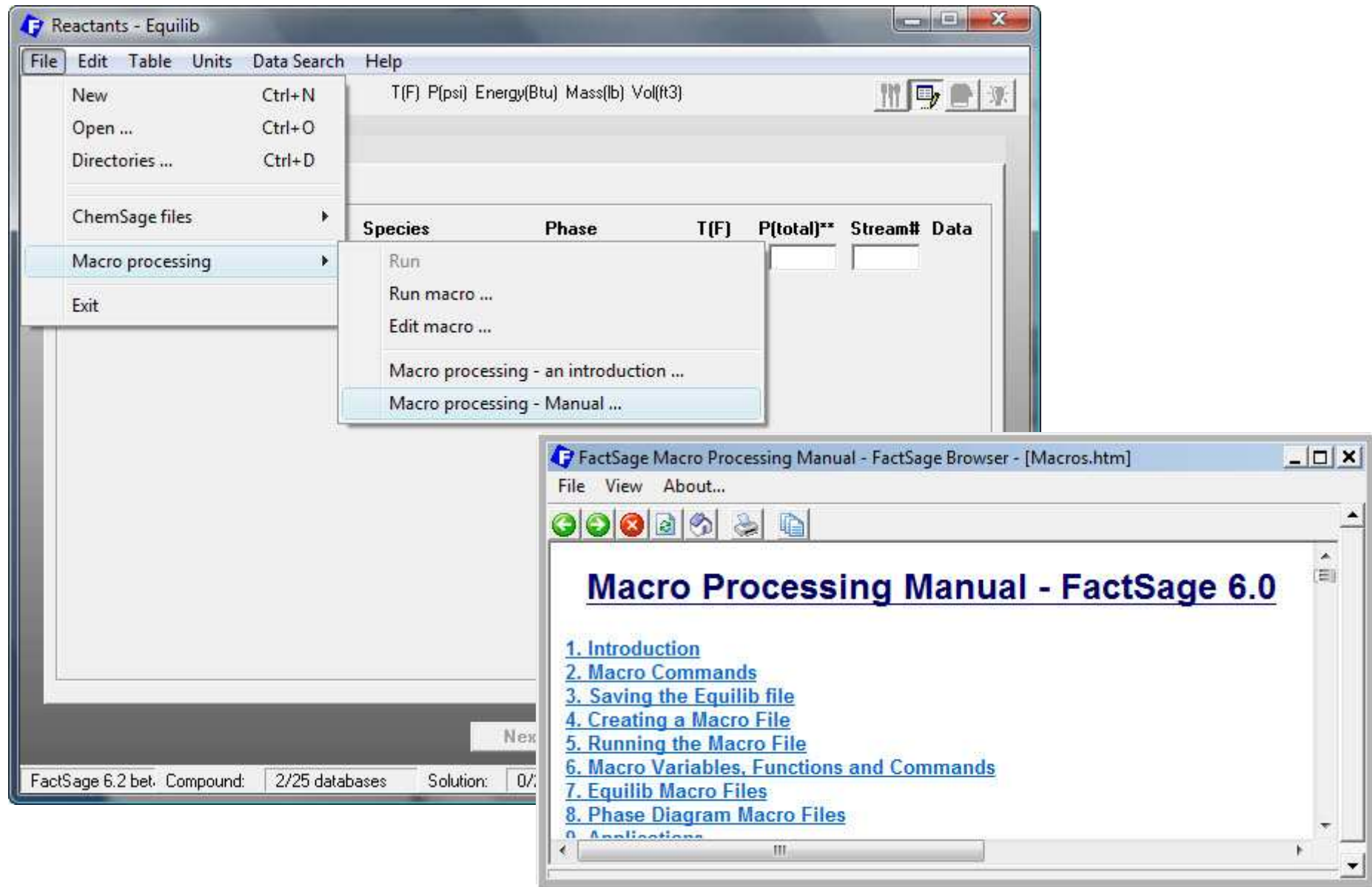
Dried Ore : 22 MgO + 46 SiO<sub>2</sub> + 31 Fe<sub>2</sub>O<sub>3</sub> + 2.672 NiO + 0.1 CoO + 1.5 C  
 Liquid Sulfur : + 1.0 S  
 HSFO + Air : + 4.6 C<sub>4</sub>H<sub>5</sub>S<sub>1</sub> + 20.7 [Air\_Real] =

100.48 litre Gas Ideal

( 45.973 vol% N<sub>2</sub>  
 + 29.233 vol% CO  
 + 15.034 vol% H<sub>2</sub>  
 + 7.0830 vol% CO<sub>2</sub>  
 + 2.4305 vol% H<sub>2</sub>O  
 + 0.19281 vol% CH<sub>4</sub>  
 + 0.48174E-01 vol% H<sub>2</sub>S  
 + 0.29676E-02 vol% COS  
 + 0.24462E-02 vol% NH<sub>3</sub>)

+ 3.2422 gram Beta\_Ni<sub>2</sub>S (Fe<sub>0.30346</sub>Ni<sub>0.37071</sub>Va<sub>0.32583</sub>)<sub>2</sub>S  
 + 0.76615 gram Pyrrhotite (Fe<sub>0.86984</sub>Ni<sub>7.6389E-2</sub>Co<sub>5.2665E-2</sub>Va<sub>1.1030E-3</sub>)S  
 + 1.2169 gram FCC 34.464 wt.% Fe + 62.184 wt.% Ni + 3.3517 wt.% Co  
 + 70.820 gram Orthopyroxene (Mg<sub>0.40234</sub>Fe<sub>0.59766</sub>){Mg<sub>0.83571</sub>Fe<sub>0.16394</sub>Fe<sup>3+</sup><sub>3.5434E-4</sub>}[Fe<sup>3+</sup><sub>3.5434E-4</sub>Si<sub>0.99965</sub>]SiO<sub>6</sub>  
 + 22.735 gram Olivine (Mg<sub>0.55007</sub>Fe<sub>0.4496</sub>Co<sub>2.0573E-4</sub>Ni<sub>1.2512E-4</sub>){Mg<sub>0.59855</sub>Fe<sub>0.3985</sub>Co<sub>1.1586E-3</sub>Ni<sub>1.7900E-3</sub>}SiO<sub>4</sub>

# Equilib – Macro Processing



# Macro Processing - Manual

**2. Macro Commands**

A macro file has 4 principal commands:

For **Equilib** calculations you can calculate an equilibrium, and then save (SAVE or SHOW) the results to a text (\*.xls) file and Xml (\*.xml) files.

For **Phase Diagram** calculations the results can be saved (SAVE and SHOW) in a figure (\*.fig) file.

Because macro processing is mainly used for the **Phase Diagram** module. Examples of Phase Diagram calculations are given in the manual.

The following 7 lines illustrate the command processing:

```
OPEN EQUI1234.DAT // Load
CALC // and
SAVE EQUI1234.TXT // Save
SHOW EQUI1234.TAB // Save
SHOW EQUI1234.XML // Save
SAVE MIXT1234.DAT GAS // Save
END // Term
```

**Summary of Macro Commands - single lines:**

|                                         |                                              |
|-----------------------------------------|----------------------------------------------|
| APPEND 'FileName' 'string'              | // Append 'string' to end of a file          |
| APPEND 'FileName1' FILENAME 'FileName2' | // Append file 'FileName2' to 'FileName1'    |
| CALC                                    | // press the F5 key                          |
| CAPTION 'string'                        | // set macro caption                         |
| CLOSE 'Filename'                        | // used with APPEND                          |
| COPY 'Source' 'Target'                  | // copy .txt, .fig, .xml files               |
| DELETE 'FileName'                       | // delete .txt, .fig, .xml files (same as K) |
| ERROROFF                                | // suppress error messages                   |
| ERRORON                                 | // resume error messages                     |
| END                                     | // last line of macro                        |
| EXIT                                    | // quit (see EXIT)                           |
| FIGURE 'Filename1.fig'                  | // display the figure                        |
| FIGURE 'Filename2.fig' SUPERIMPOSE      | // superimpose the figure                    |
| HIDE                                    | // hide FactSage window                      |
| HIDEMACRO                               | // hide the macro window                     |
| IF 'Value1' = [< > =< >] 'Value2'       | // 'IF' statement                            |

**Summary of \$Thermochemical\$ Variables: \$E\_\*\$, \$M\_\*\$, \$R\_\*\$, \$U\_\***

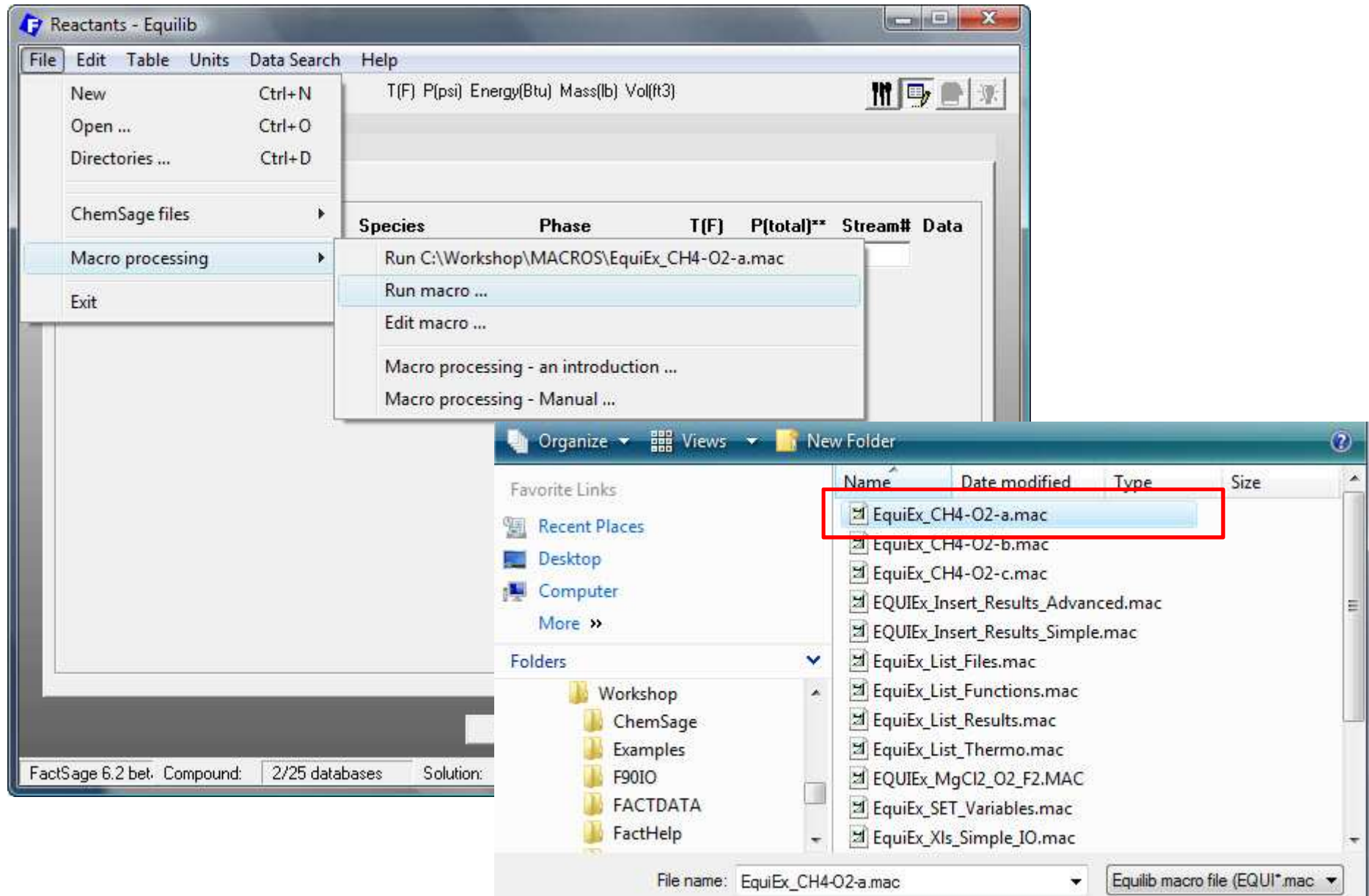
Thermochemical variables are case sensitive and system dependent. They are defined by the Equi\*.dat (or calculated during the equilibrium calculation ("CALC") and can not be modified by you (except by editing the Phas\*.dat file) - see the 'SET' macro command for the thermochemical variables that you can modify.

An example of the common thermochemical variables is given in the macro file 'EquiEx\_List\_Results.mac'. An example of most calculated thermochemical variables including solution integral and partial properties and c is given in the macro file 'EquiEx\_List\_Thermo.mac'. An example of the 'SET' command is given in 'EquiEx\_SET\_Variables.mac'.

**Legend:** - note, all thermochemical variables are case sensitive.

- A = Alpha
- a = activity
- B = Beta
- C = Cp heat capacity
- c = compound (pure substance) or molar cp
- D = data source
- E = extended name (data source and name)
- e = elements (+ electron phases) i.e. components
- F = total Gibbs free energy
- f = molar Gibbs free energy
- g = grams
- h = molar enthalpy
- H = total enthalpy
- i = integer
- i = integer

# Equilib – running a macro



# Macro processing – Excel i/o : maximum flame temperature

The screenshot shows an Excel spreadsheet with columns A-F and rows 22-47. The spreadsheet contains data for calculating the maximum flame temperature based on the equivalence ratio (Alpha). The 'Macro' window shows the execution of a VBA script that writes the current Alpha value to a file and displays a message box. The 'Results - Equilib' window shows the output of the FactSage calculation for the current Alpha value.

| Alpha  | DeltaH | Temperature | T(change) | Alpha(inc) |
|--------|--------|-------------|-----------|------------|
| 0.6    | 0      | 2757.36     | 2757.36   | 0.01       |
| 0.61   | 0      | 2768.59     | 11.23     | 0.01       |
| 0.62   | 0      | 2776.55     | 7.96      | 0.01       |
| 0.63   | 0      | 2781.66     | 5.11      | 0.01       |
| 0.64   |        |             |           | 0.01       |
| 0.65   |        |             |           | 0          |
| 0.66   |        |             |           | 0          |
| 0.643  | 0      | 2784.63     | 9.00E-02  | 0.0        |
| 0.644  | 0      | 2784.7      | 0.07      | 0.0        |
| 0.645  | 0      | 2784.76     | 6.00E-02  | 0.0        |
| 0.646  | 0      | 2784.79     | 3.00E-02  | 0.0        |
| 0.647  | 0      | 2784.8      | 1.00E-02  | 0.0        |
| 0.648  | 0      | 2784.79     | -1.00E-02 | 0.0        |
| 0.646  | 0      | 2784.79     | 2784.79   | 0.00       |
| 0.6461 | 0      | 2784.79     | 0         | 0.00       |

**Reactants - Equilib**  
T(max) = 2784.79 at <Alpha> = 0.646

**Macro**  
-----> WRITE ->  
00:00:51 IF 0 <= 0 GOTO CheckAnswer  
00:00:51 MARK CHECKANSWER  
00:00:51 IF 0.0001 = 0.0001 GOTO QUIT  
00:00:51 MARK QUIT  
00:00:51 SHOW  
00:00:51 MSGBOX T(max) = 2784.79 at <Alpha> = 0.646  
00:03:17 SHOW EQUIE<sub>x</sub>\_CH4-O2.txt  
00:03:44 END ... macro processing terminated.

**Results - Equilib 2784.79 C FactSage 6.2 beta**  
Output Edit Show Pages  
T(C) P(atm) Energy(J) Mass(mol) Vol(litre)  
(25, 1, g, #1) (25, 1, g, #1)  
1.2691 mol gas\_ideal  
(26.352 gram, 1.2691 mol, 318.44 litre, 8.2752E-05 g/ml)  
(2784.79 C, 1 atm, a=1.0000)  
( 0.39620 H2O  
+ 0.17357 CO  
+ 0.10530 CO2  
+ 8.9519E-02 H2  
+ 8.8009E-02 OH  
+ 5.8354E-02 O2  
+ 5.5960E-02 H  
+ 3.3034E-02 O  
+ 5.4536E-05 HOO  
+ 1.6889E-06 HOOH  
+ 7.0645E-07 HCO  
+ 1.5292E-08 O3  
+ 8.9138E-09 H2CO  
+ 1.0625E-10 HCOOH  
+ 2.7813E-11 C