Processing - Combustion and Heat

1. Introduction to combustion
2. Compound databases : FactSage Browser & View Data - FACT53, SGPS
3. Simple combustion : $CH_4 + 2O_2 => CO_2 + 2H_2O$ – isothermal, adiabatic
4. Combustion in air : <Alpha> variable <1-A> CH_4 + <0.21A> O_2 + <0.79A> N_2
5. Real air and non-ideal calculations
6. Private compound data : ‘coke’, ‘anthracite’ and HSFO ‘high sulfur fuel oil’ data –combustion calculations
7. Equilibria : reduction kiln - pre-reduction of the Ni ore by ‘coke’ and ‘HSFO’
8. Macro processing : Excel i/o - maximum flame temperature

Introduction to combustion

Definition of combustion or burning:
fuel + oxidant => product species + exothermic heat

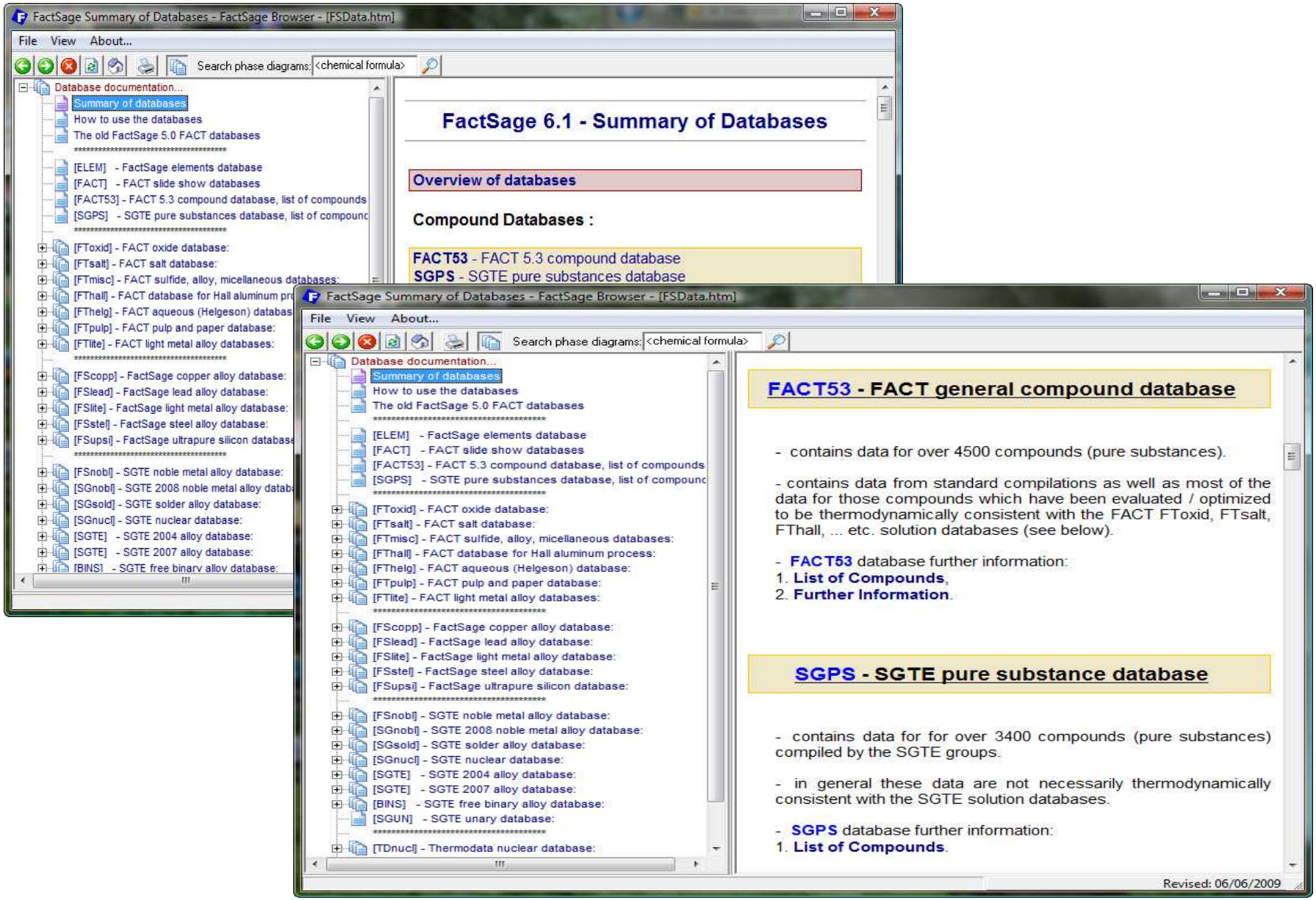
Fuels often include organic compounds (especially hydrocarbons) in the gas, liquid or solid phase. Combustion reactions can be slow burning or rapid explosions

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

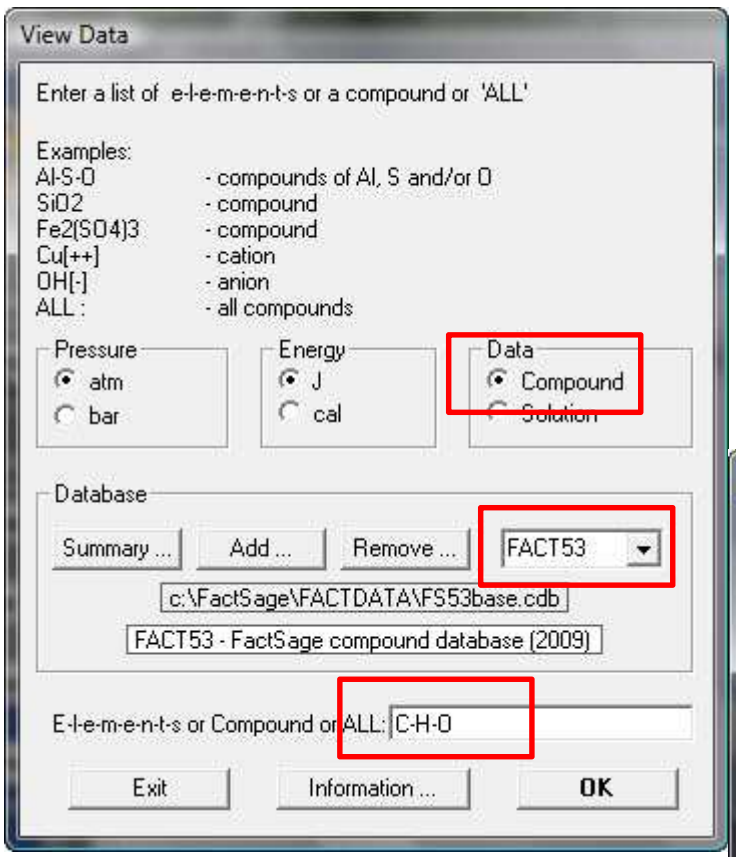
carbon: $C(s) + O_2 \Rightarrow CO_2$
hydrogen: $H_2 + 0.5\ O_2 \Rightarrow H_2O$
methane: $CH_4 + 2\ O_2 \Rightarrow CO_2 + 2\ H_2O$
butane: $C_4H_{10} + 6.5\ O_2 \Rightarrow 4\ CO_2 + 5\ H_2O$
acetylene: $C_2H_2 + 2.5\ O_2 \Rightarrow 2\ CO_2 + H_2O$
kerosene: $C_{12}H_{26}(l) + 18.5\ O_2(l) \Rightarrow 12\ CO_2 + 13\ H_2O$
thioformaldehyde: $CH_2S + 6\ F_2 \Rightarrow CF_4 + 2HF + SF_6$

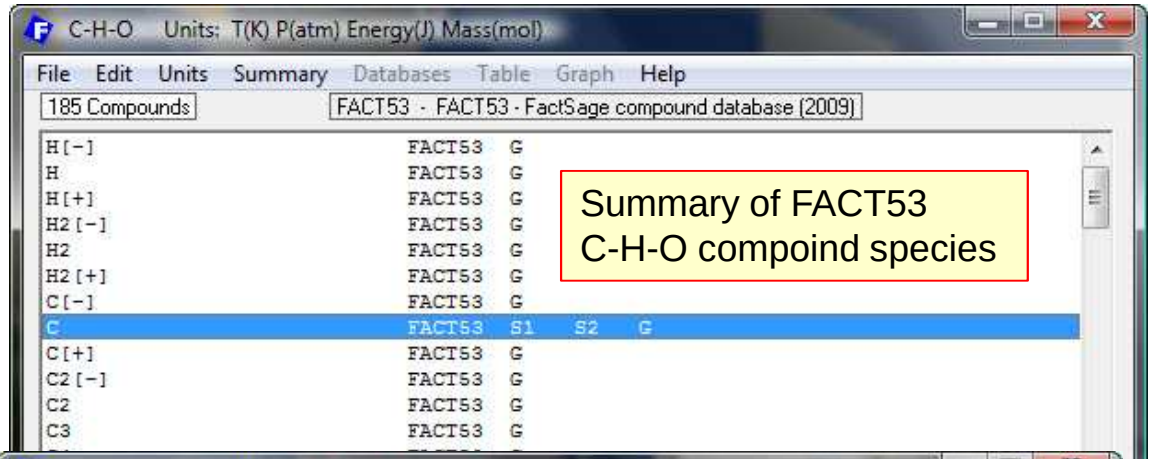
None of the combustion reactions are stoichiometric as written above - product gases form complex chemical equilibria with O, O_3, OH, H^+, e^- etc. especially at high temperatures.

FactSage Browser - compound databases FACT53, SGPS

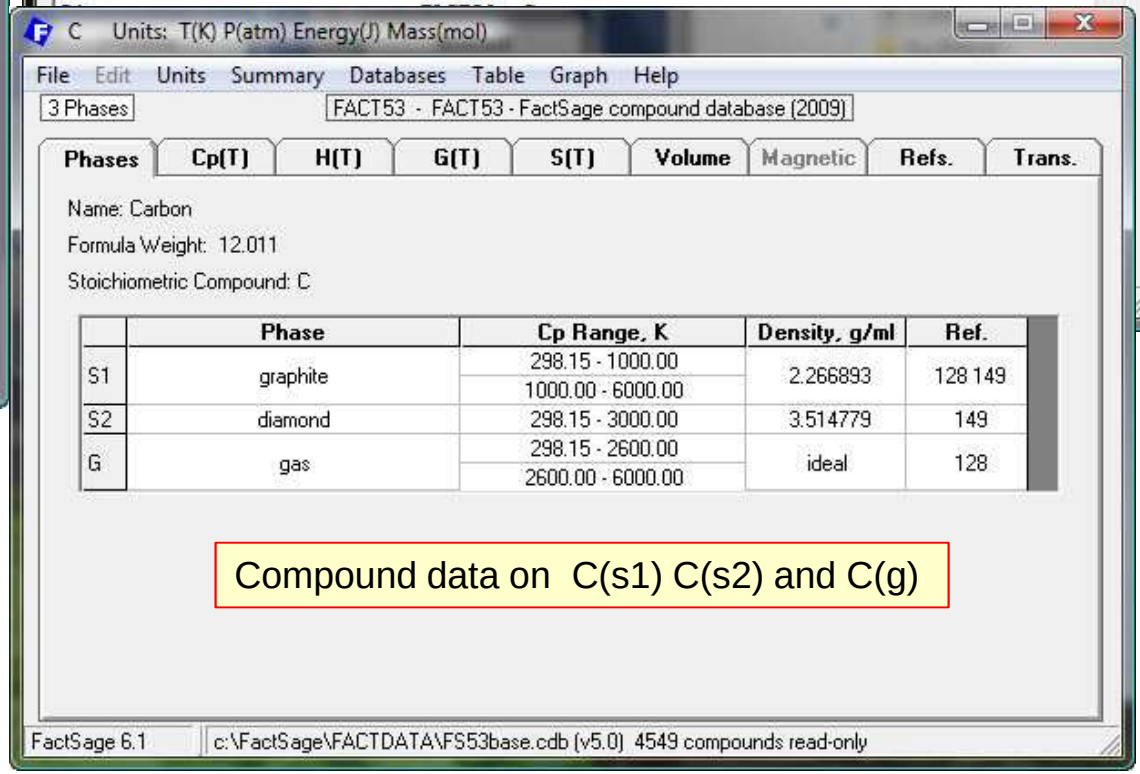


View Data - compound databases FACT53, SGPS





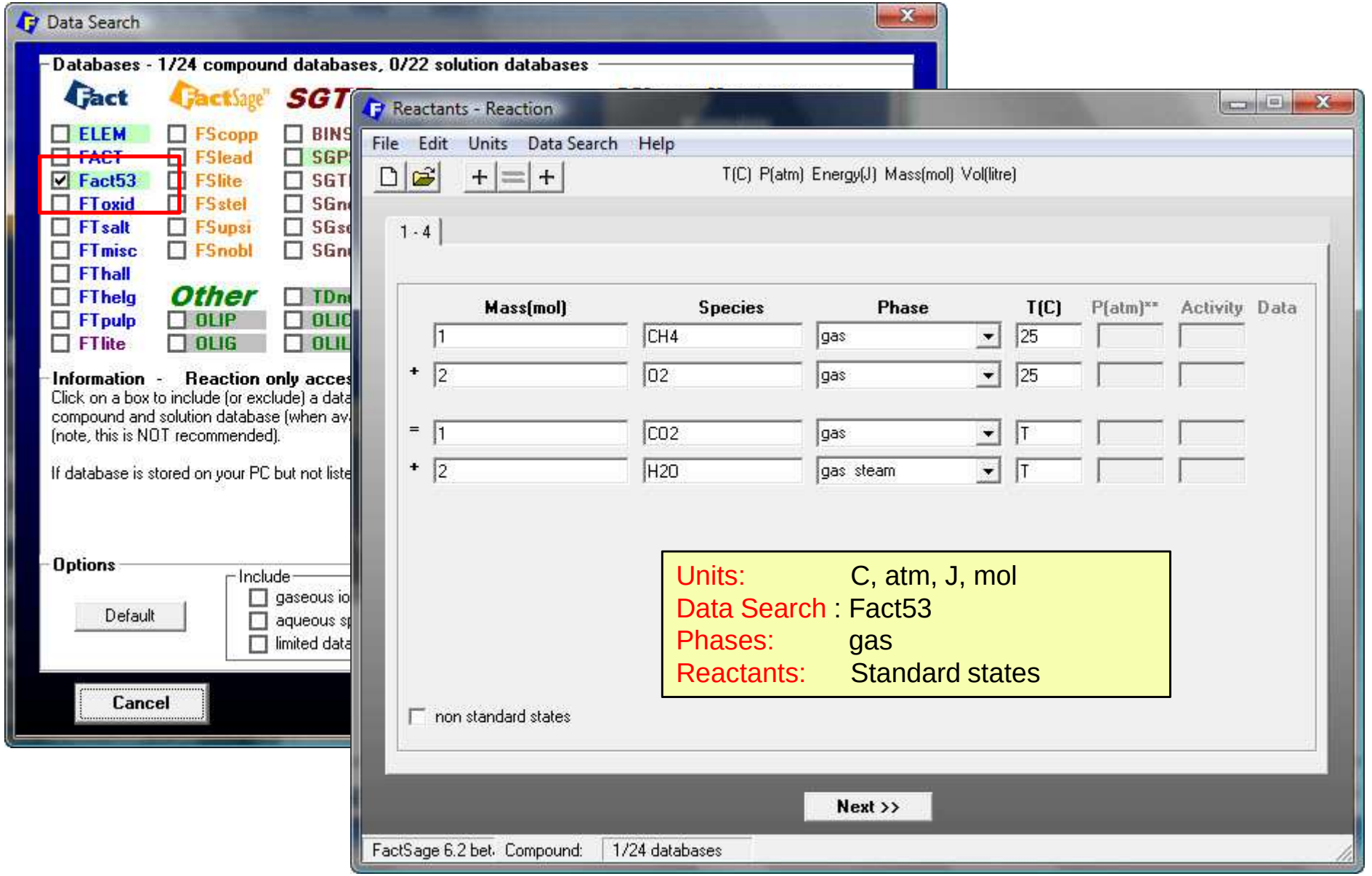
Summary of FACT53
C-H-O compoind species



Compound Database : FACT53
Elements : C-H-O

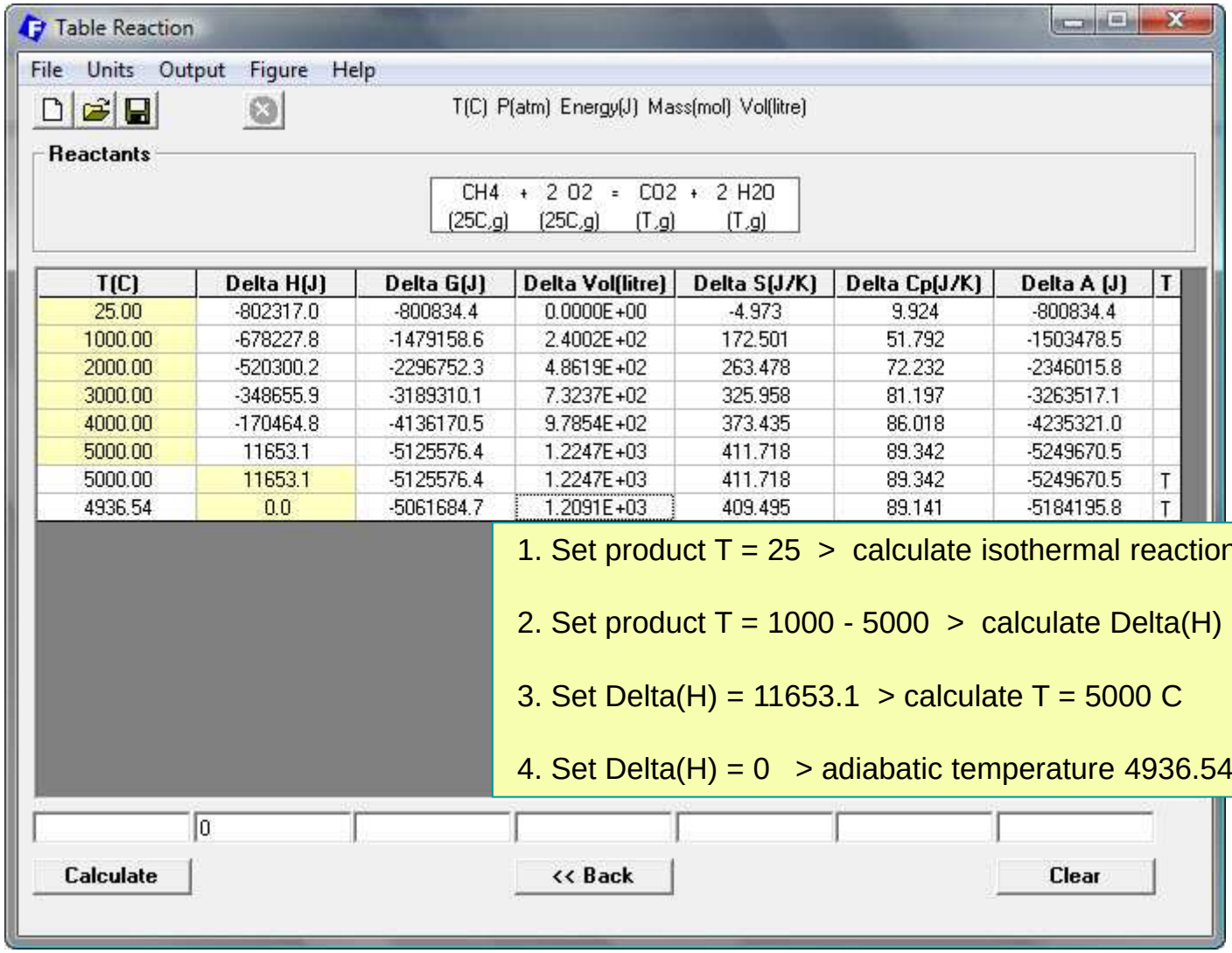
Compound data on C(s1) C(s2) and C(g)

Reaction – Simple Combustion



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

Reaction – Simple Combustion



1. Set product T = 25 > calculate isothermal reaction

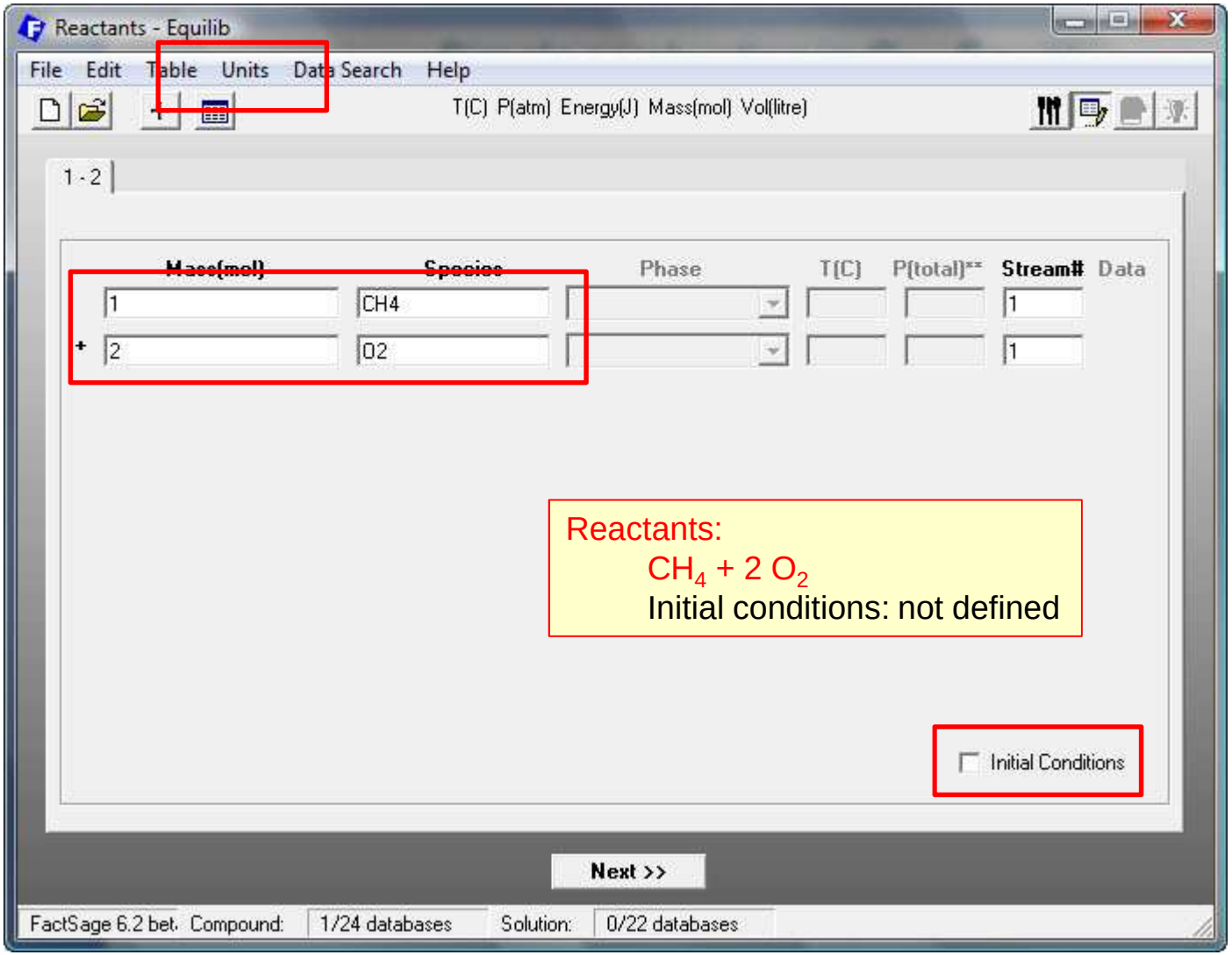
2. Set product T = 1000 - 5000 > calculate Delta(H) at T

3. Set Delta(H) = 11653.1 > calculate T = 5000 C

4. Set Delta(H) = 0 > adiabatic temperature 4936.54 C

Equilib – Simple Combustion

Units: C, atm, J, mol

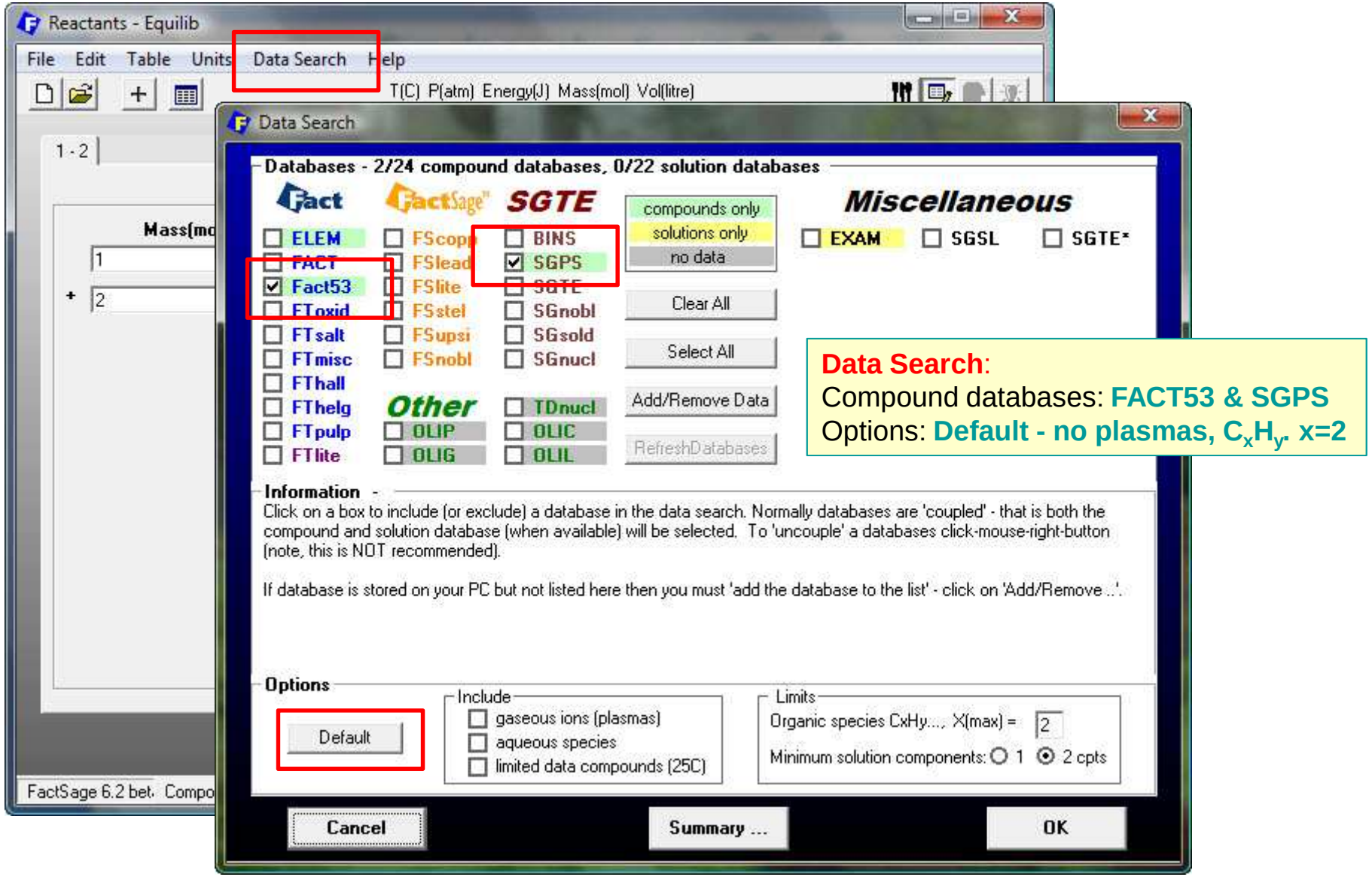


Reactants:

$CH_4 + 2\ O_2$

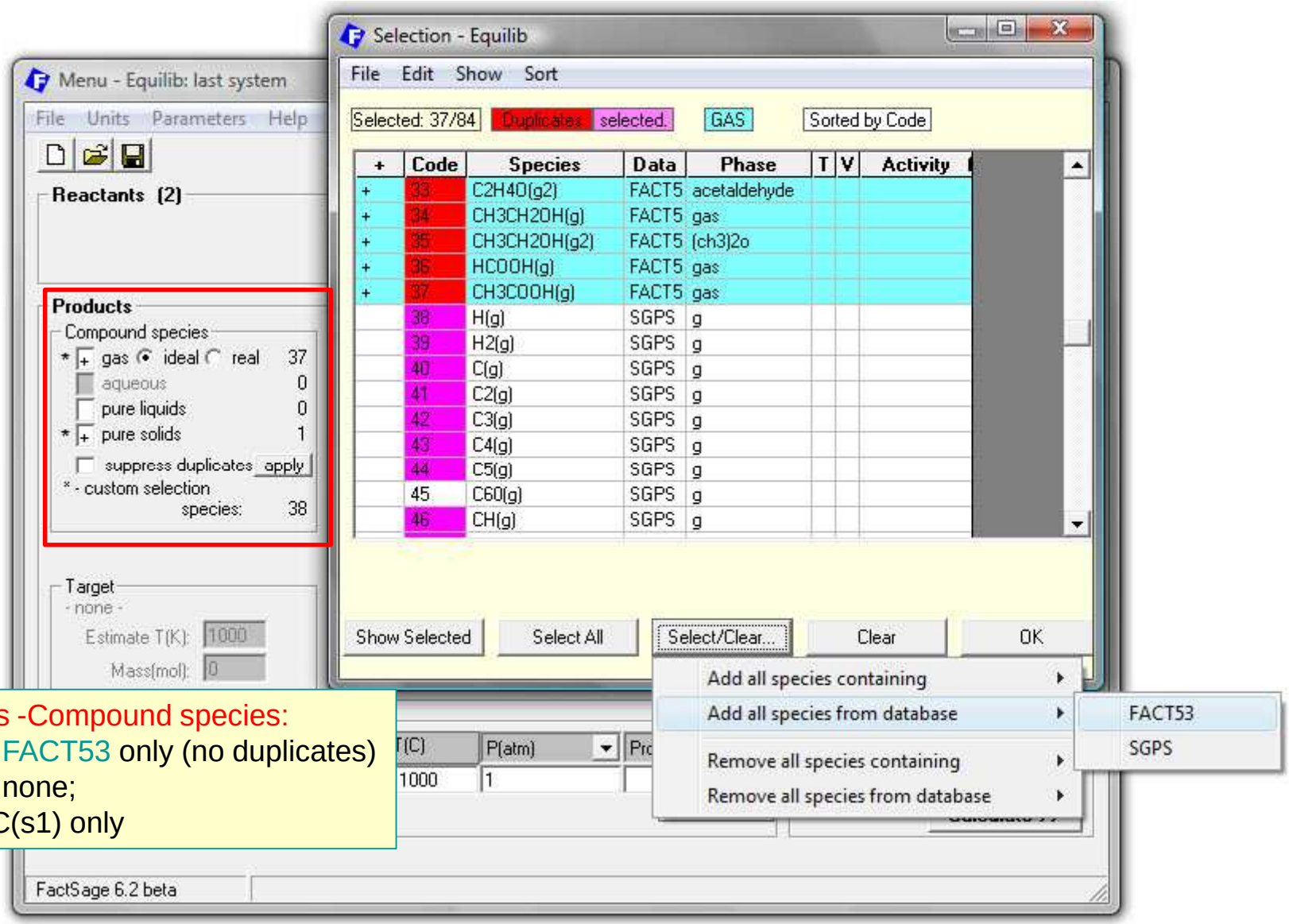
Initial conditions: not defined

Equilib - Data Search



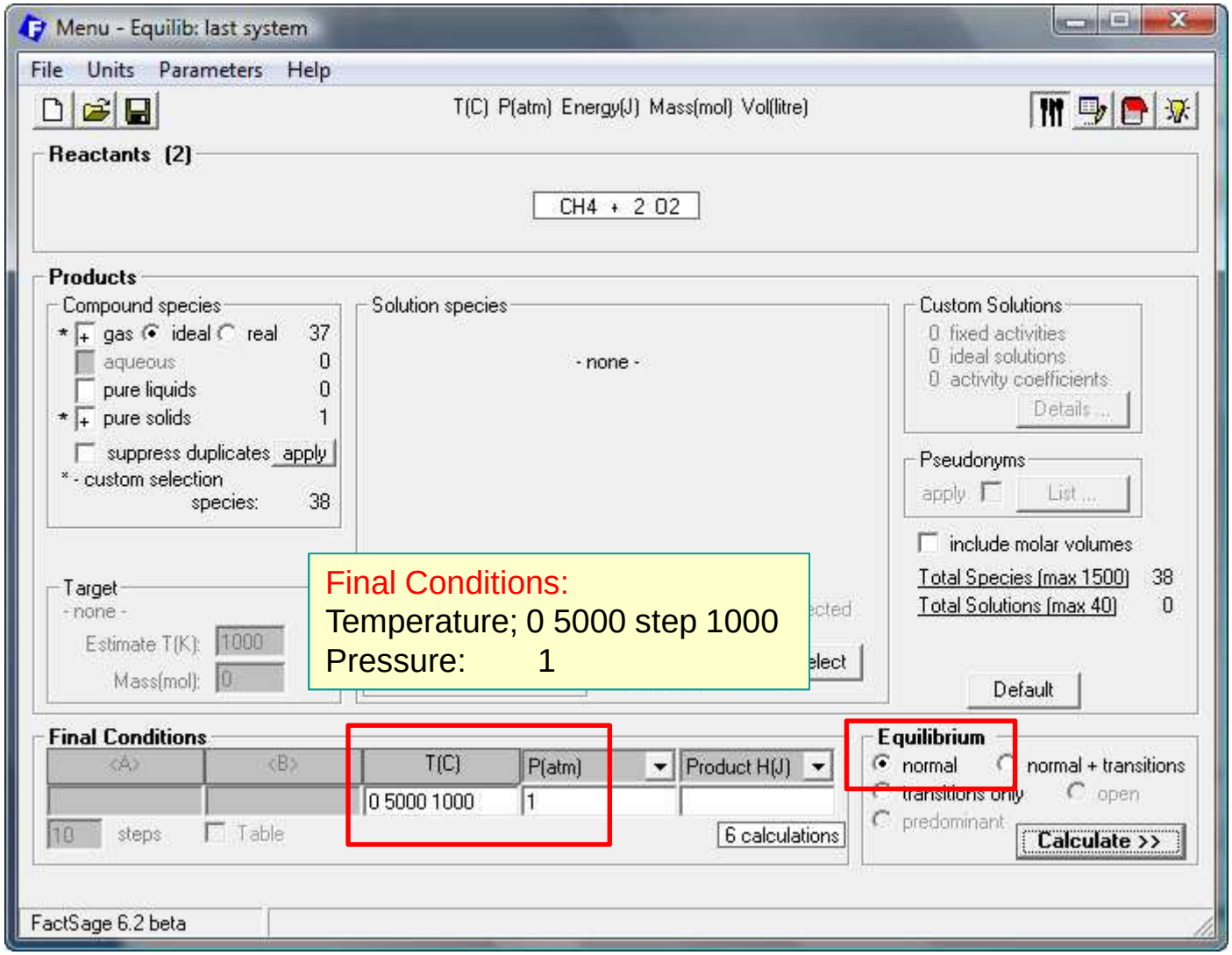
Data Search:
Compound databases: **FACT53 & SGPS**
Options: **Default - no plasmas, C_xH_y. x=2**

Equilib Selection Window – simple combustion

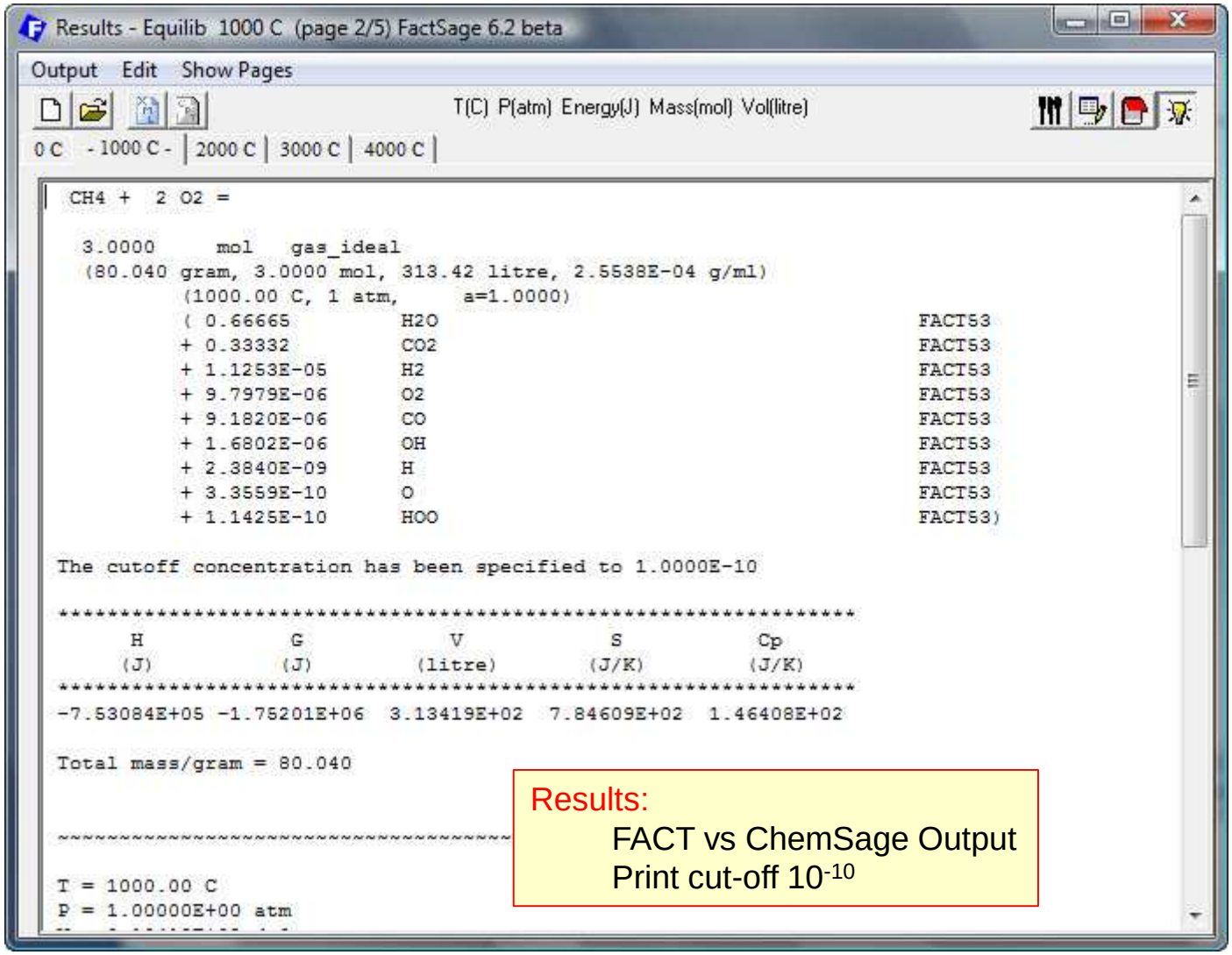


Products -Compound species:
Gases : FACT53 only (no duplicates)
Liquids: none;
Solids: C(s1) only

Equilib Menu Window – simple combustion



Equilib Results Window – FACT output

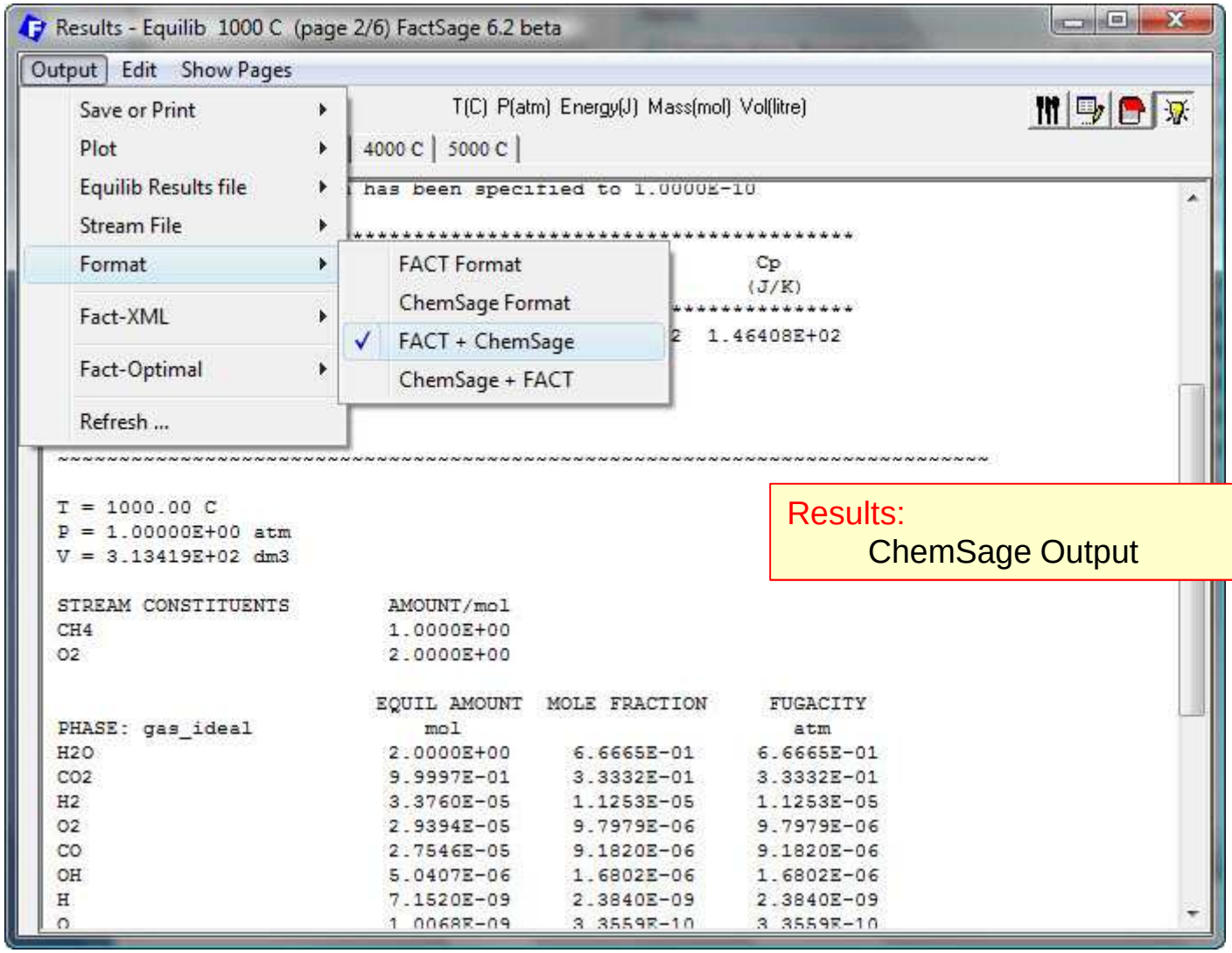


Results:

FACT vs ChemSage Output

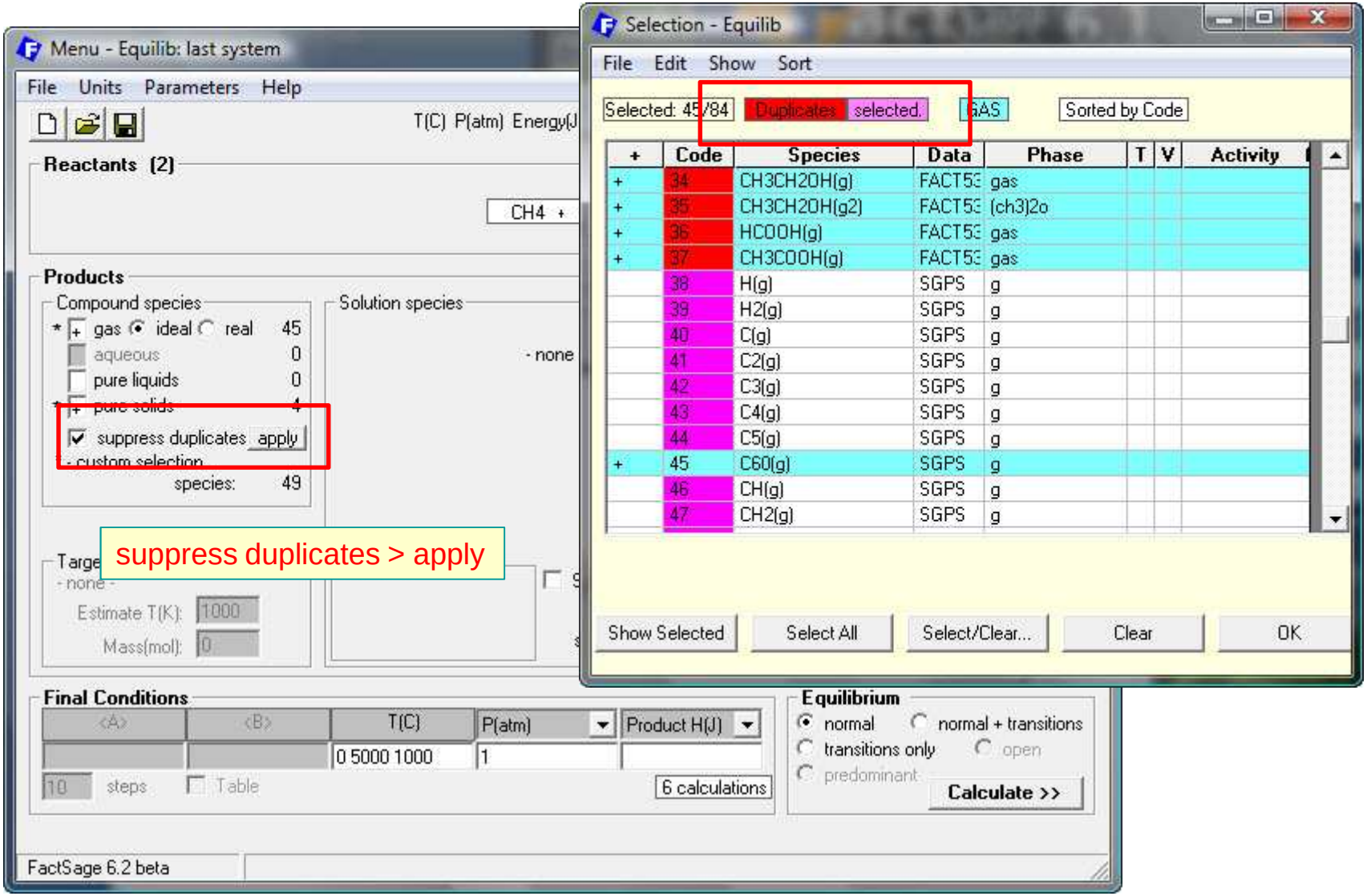
Print cut-off 10^{-10}

Equilib Results Window – Chemsage output

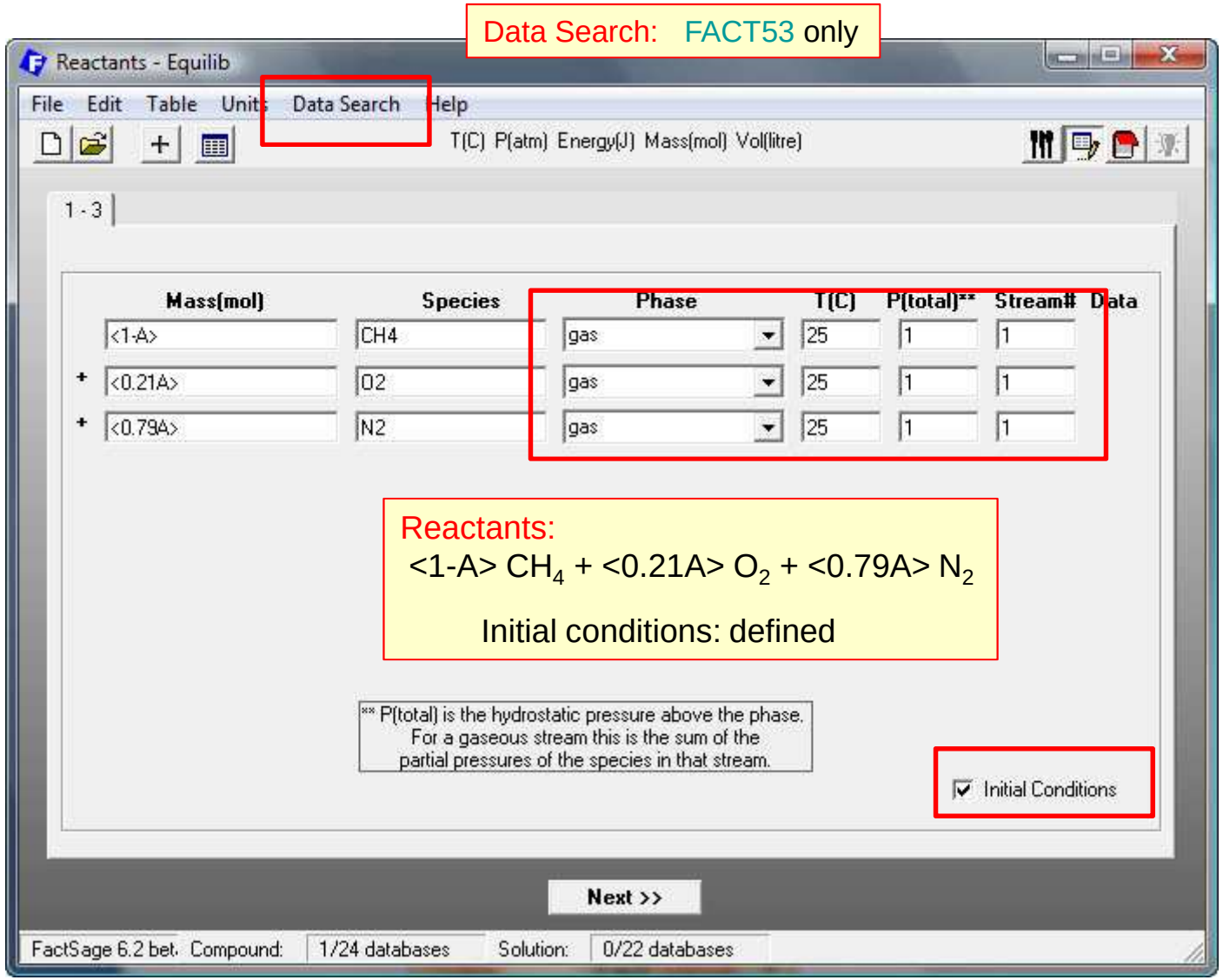


Results:
ChemSage Output

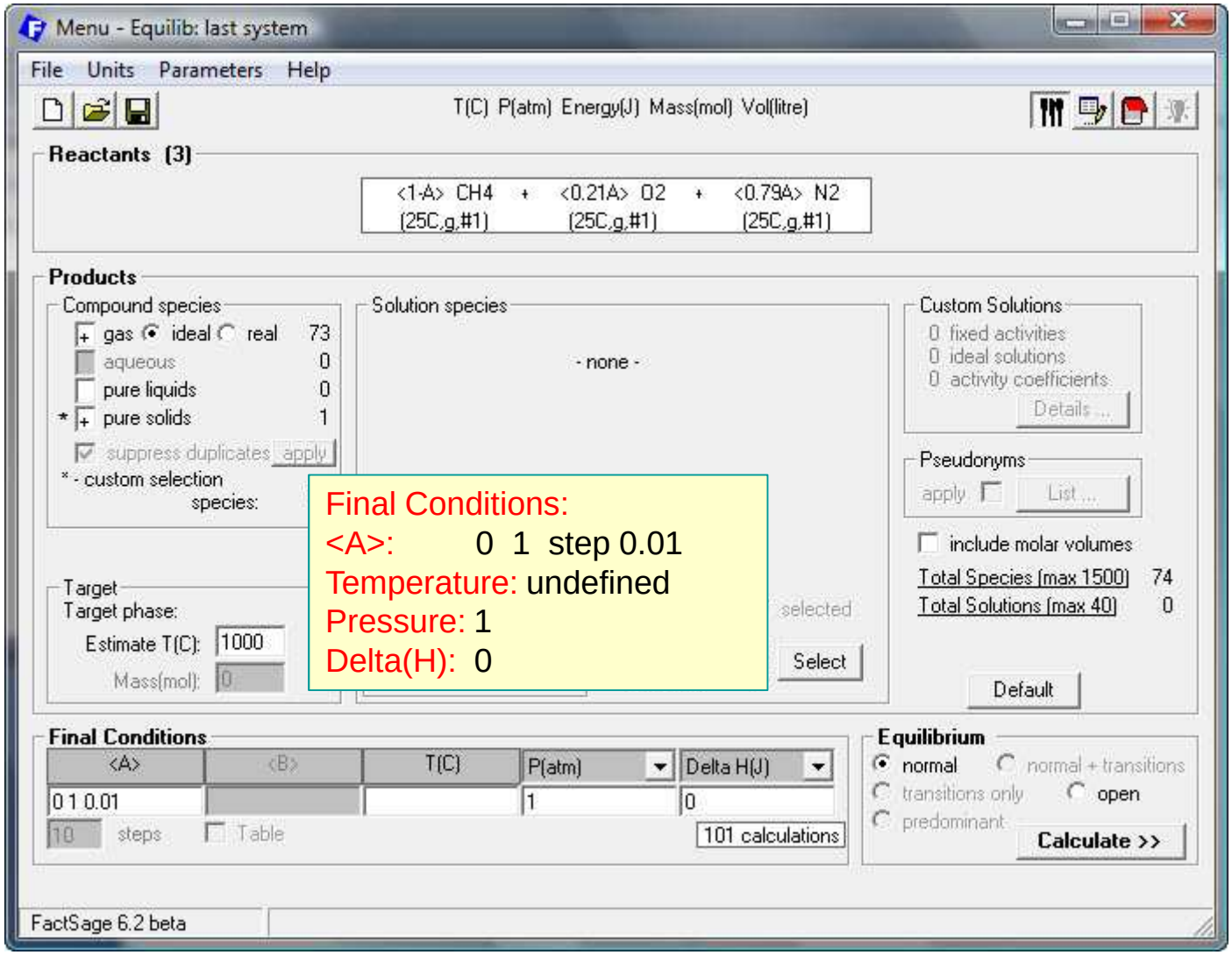
Equilib – Duplicate data in Fact53 & SGPS



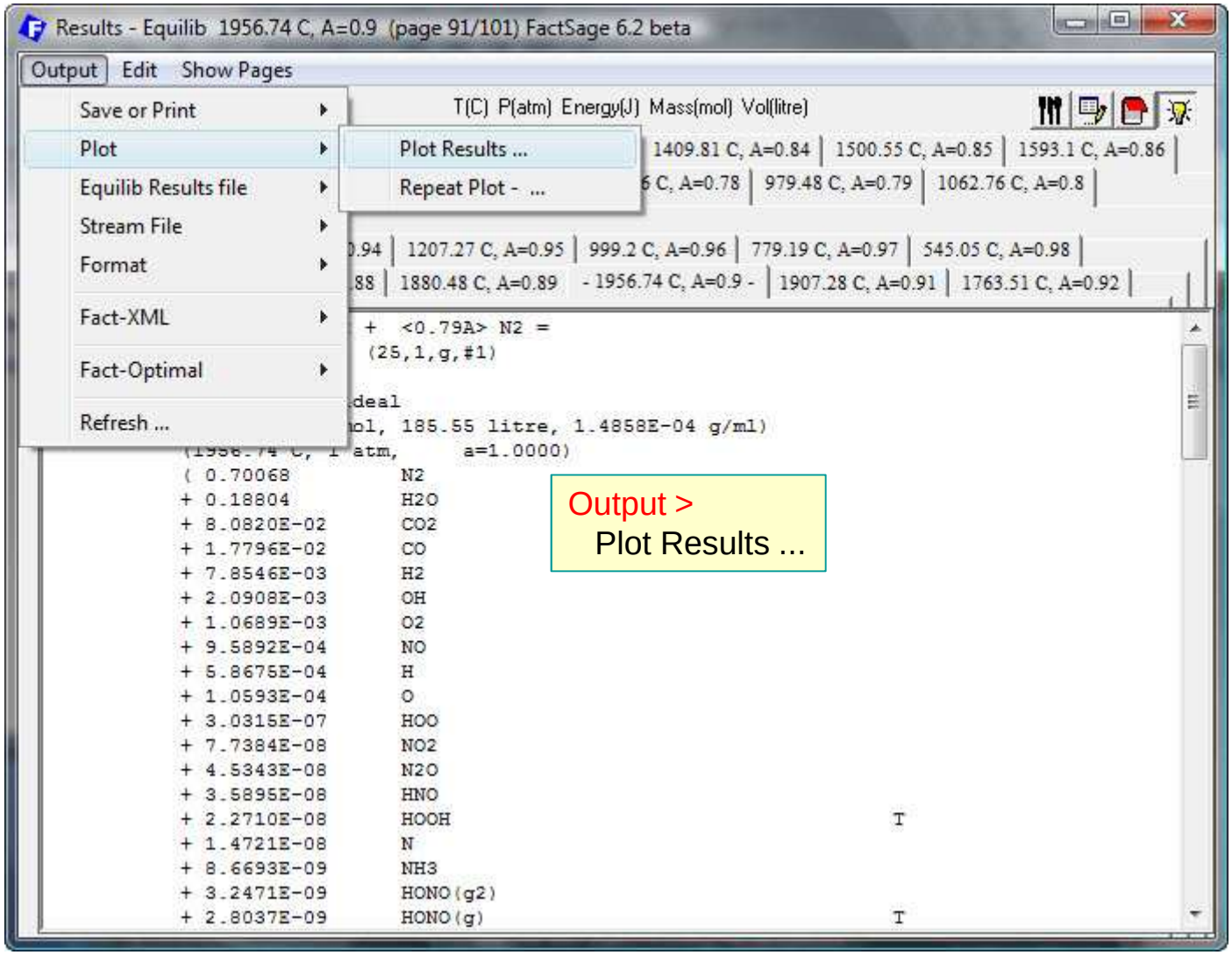
Equilib Reactants Window – combustion in air



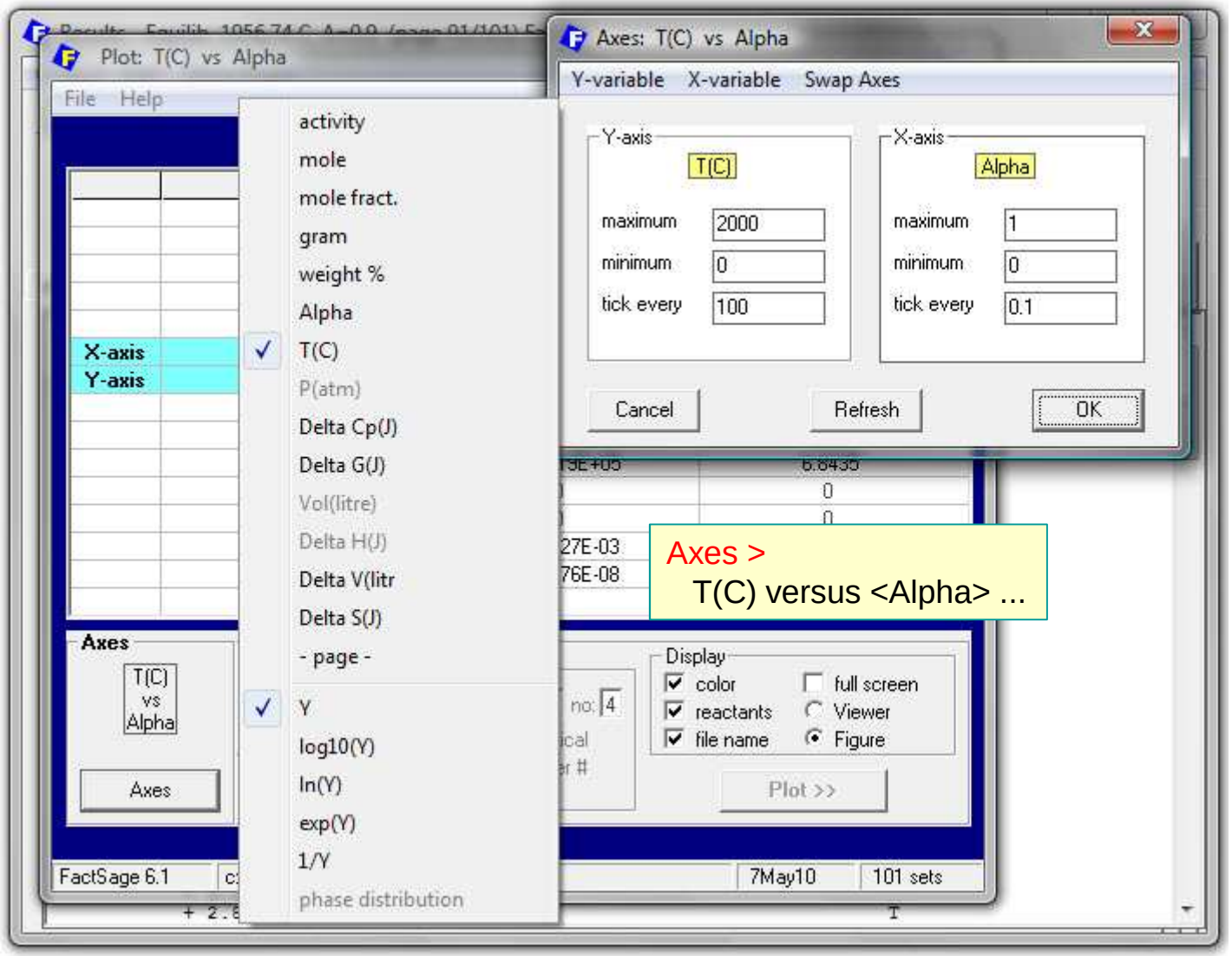
Equilib Menu Window – combustion in air



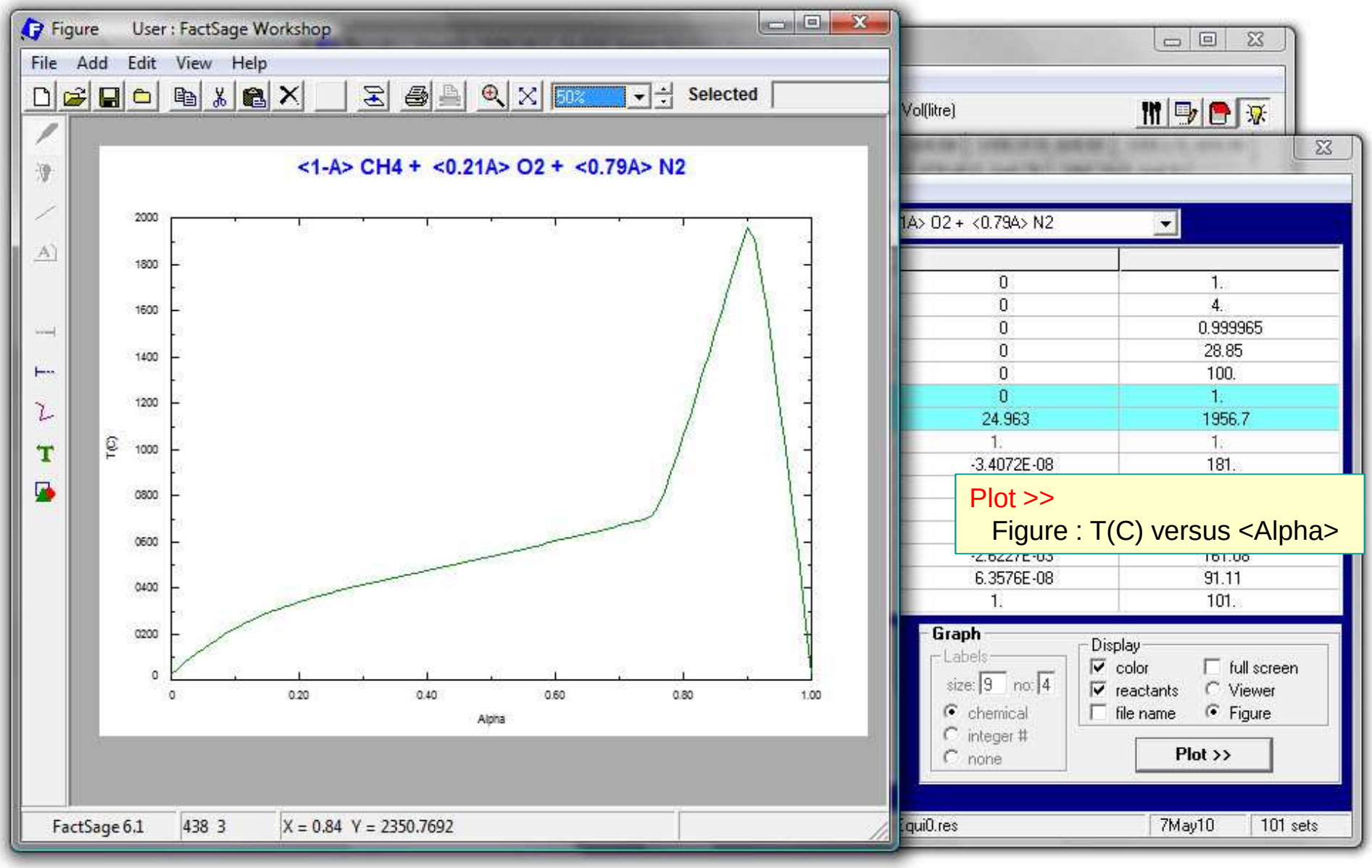
Equilib Results Window – combustion in air



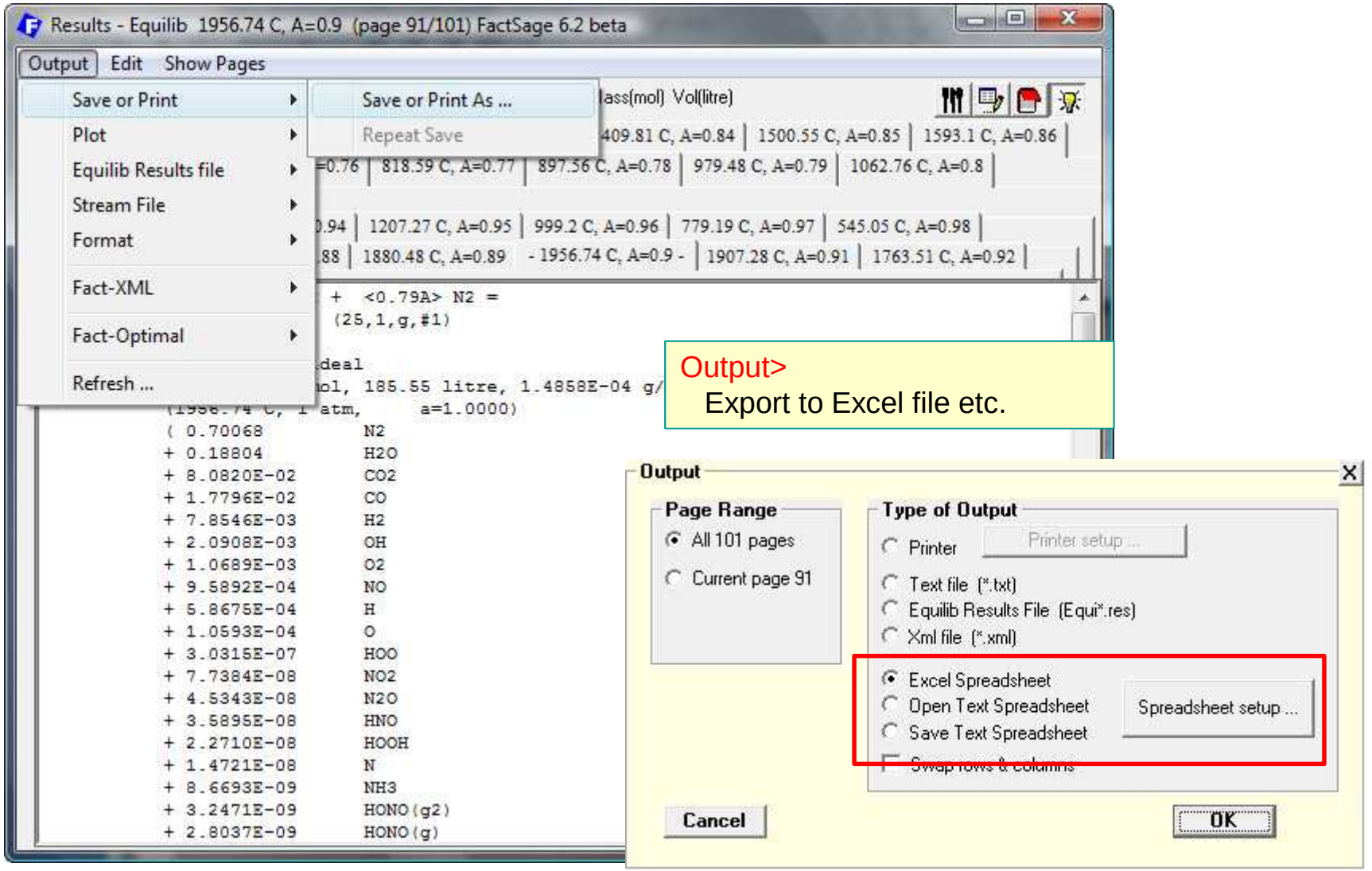
Equilib Results Window - combustion in air - plot results



Equilib Results Window - combustion in air - plot results

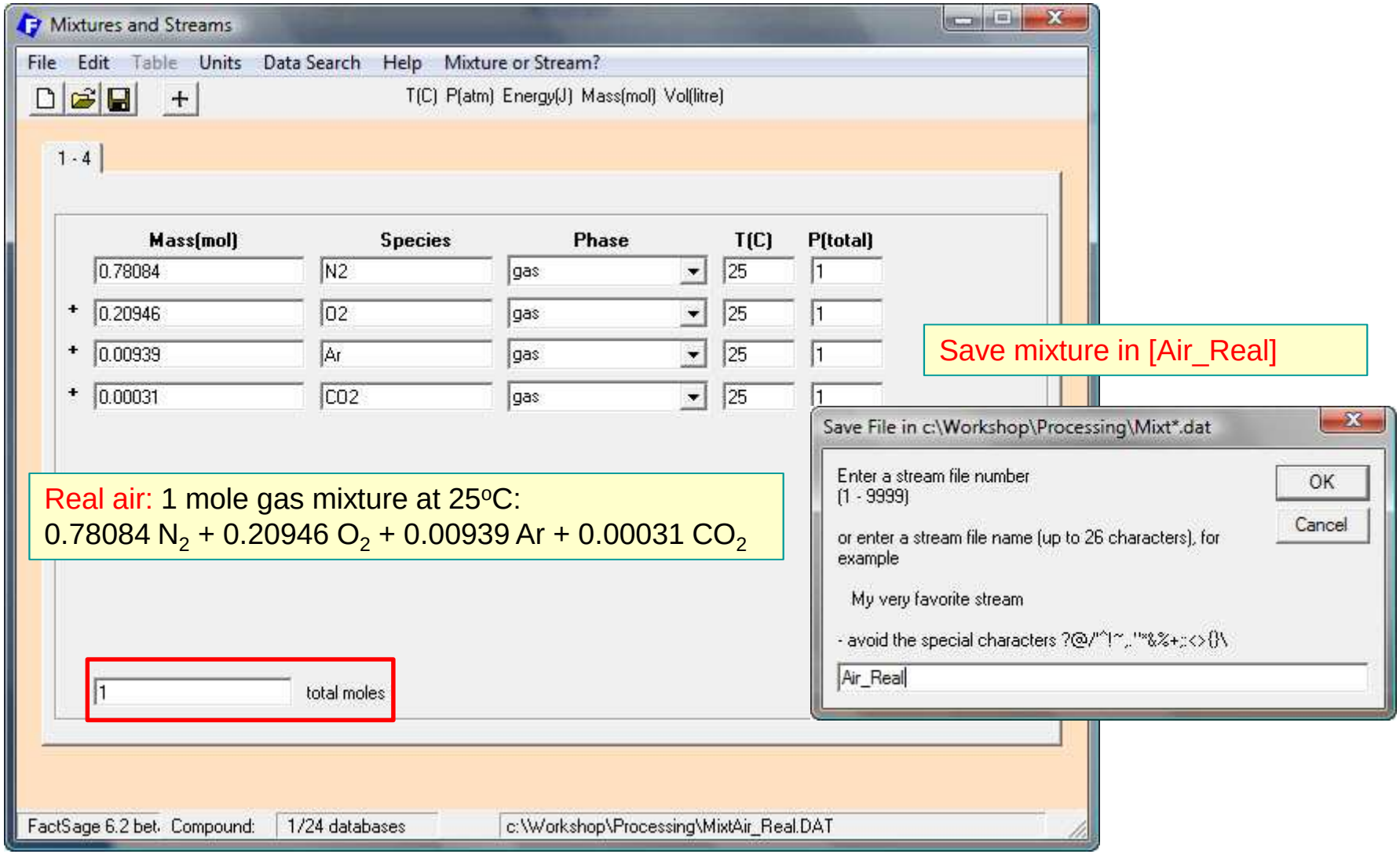


Equilib Results Window - export results to Excel

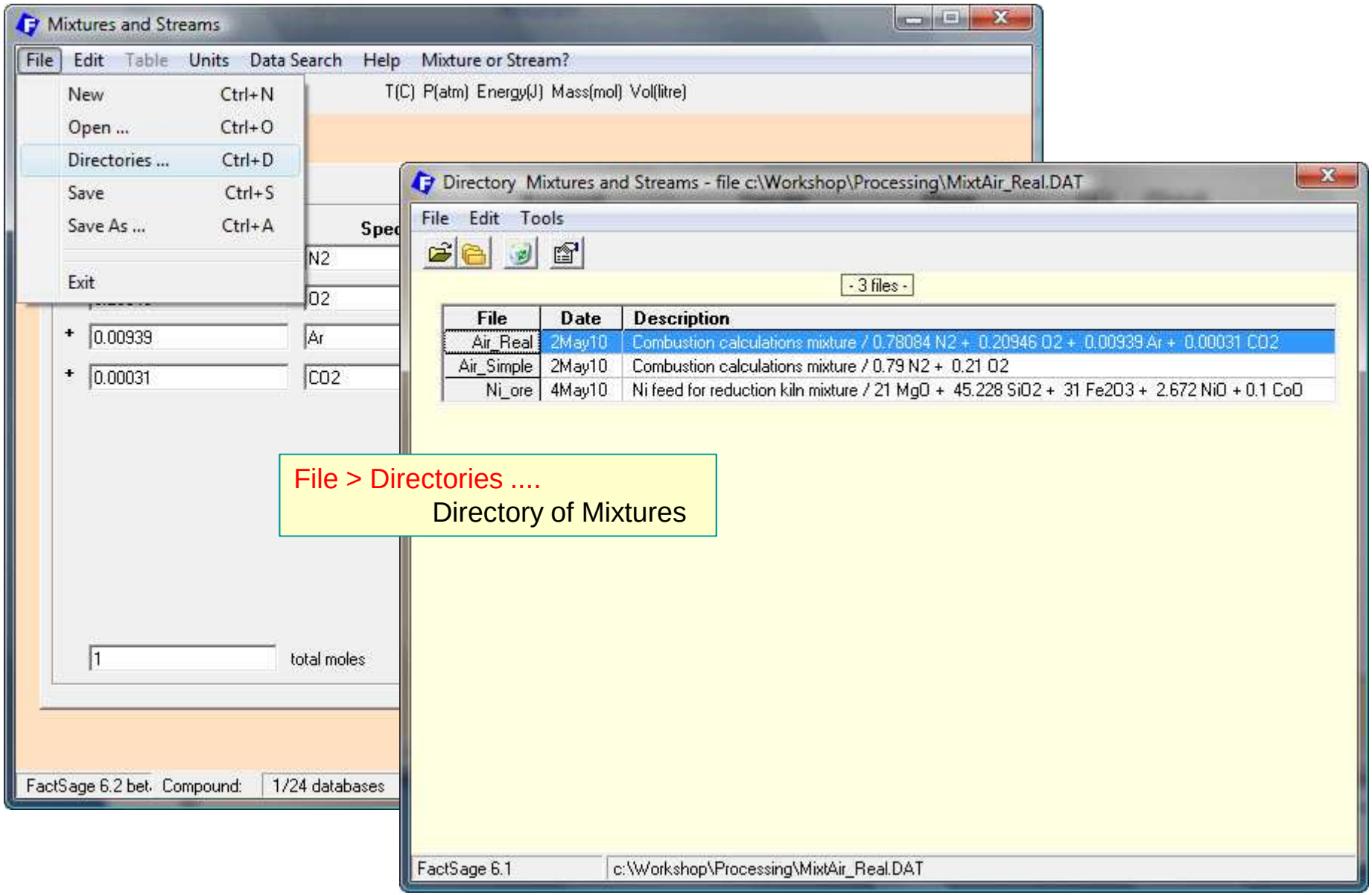


Mixtures – Mixture Module

Mixtures – real air

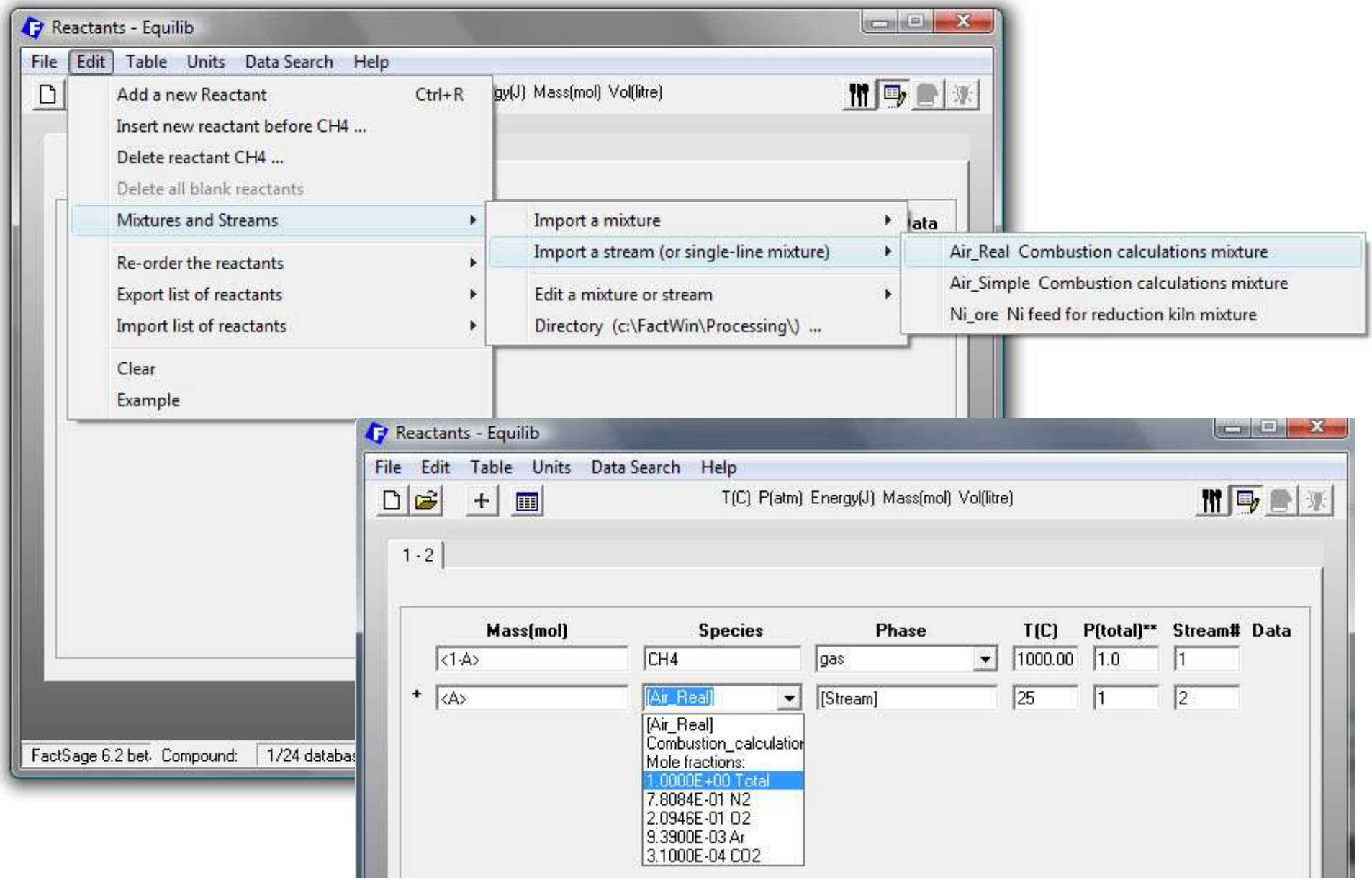


Mixtures – real air

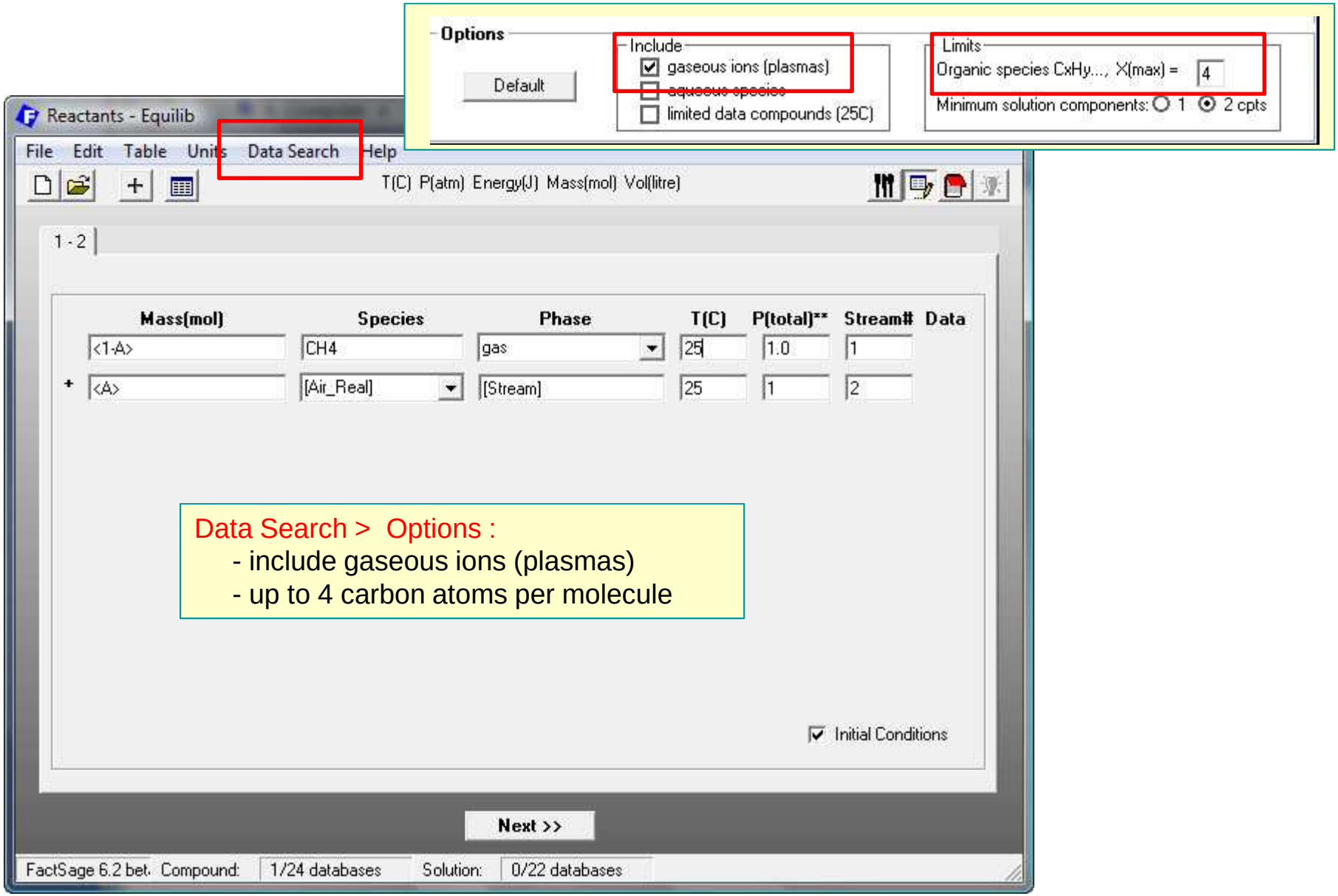


File > Directories ....
Directory of Mixtures

Mixtures – importing [Air_Real] mixture into Equilib



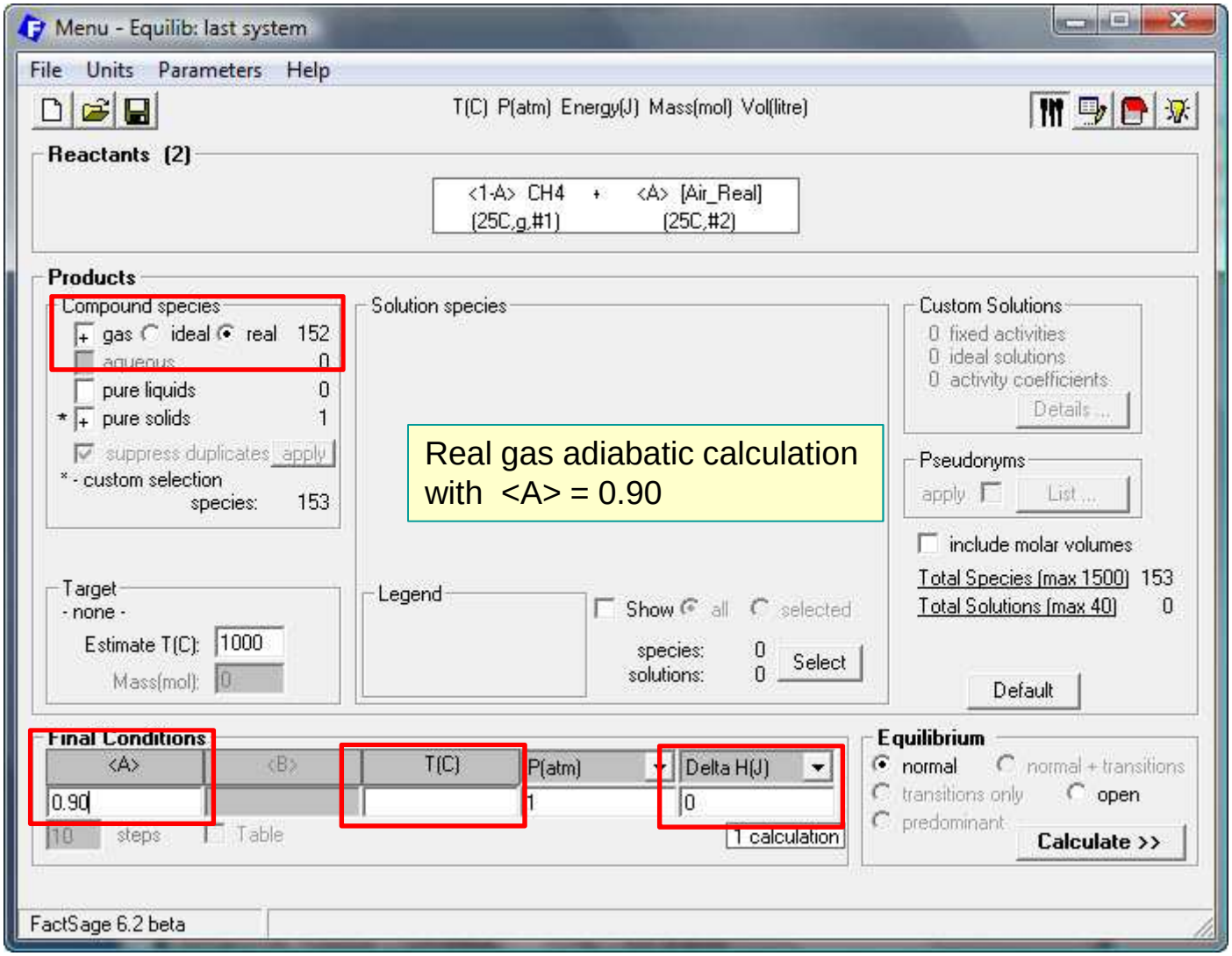
Equilib – Data Search options



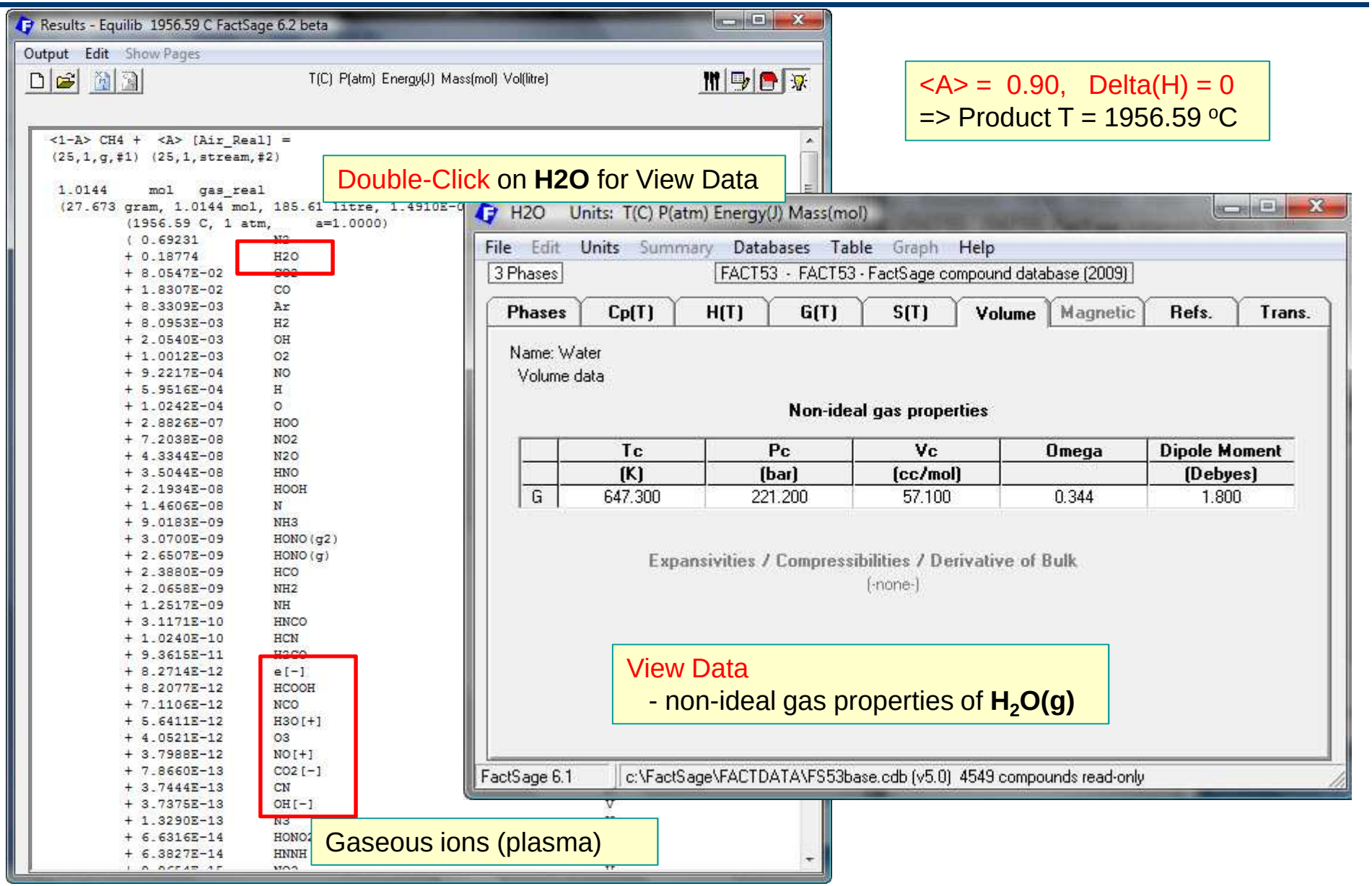
Data Search > Options :

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

Equilib Menu Window – real gas adiabatic settings



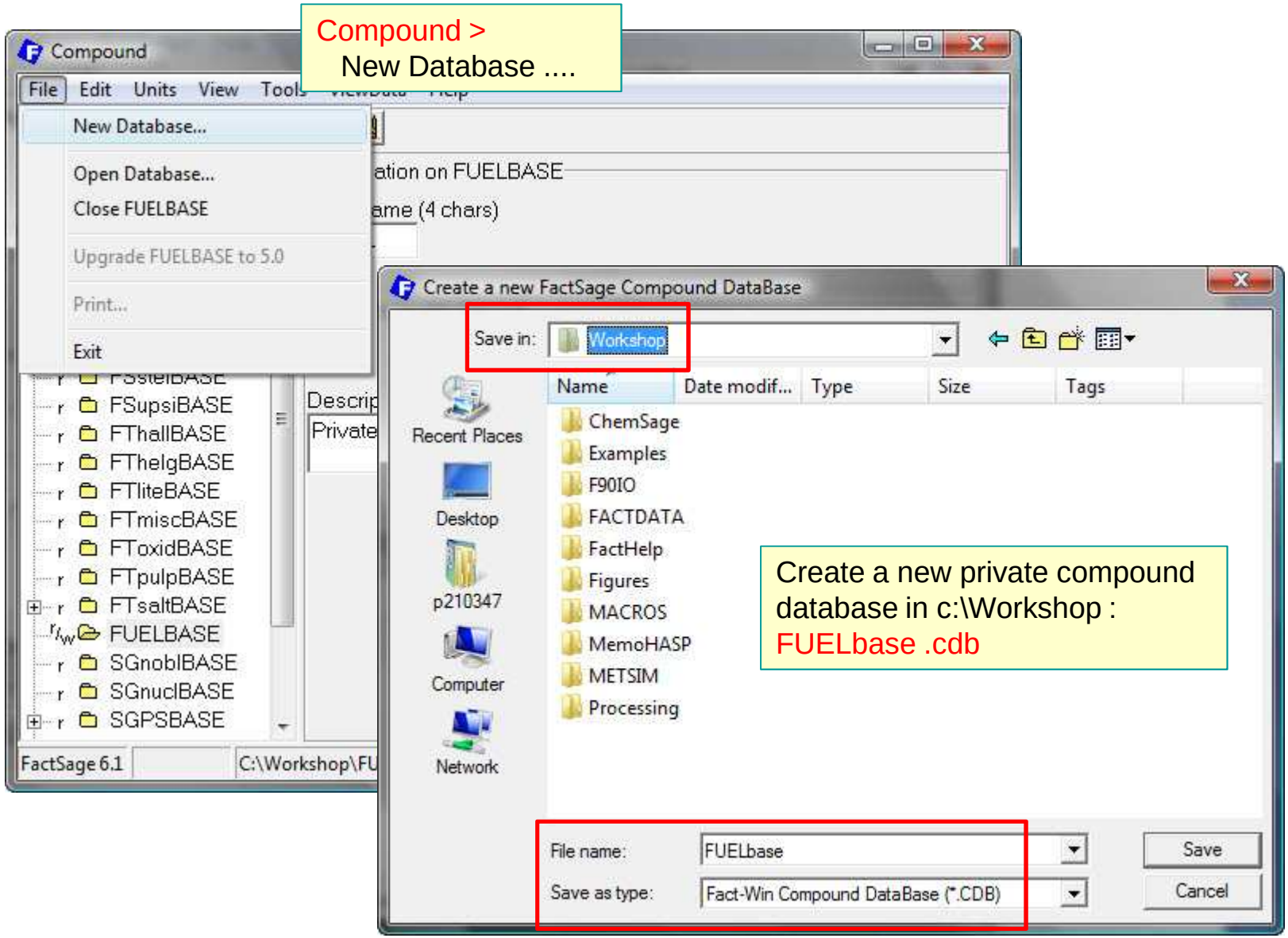
Equilib Results Window – real gas adiabatic temperature



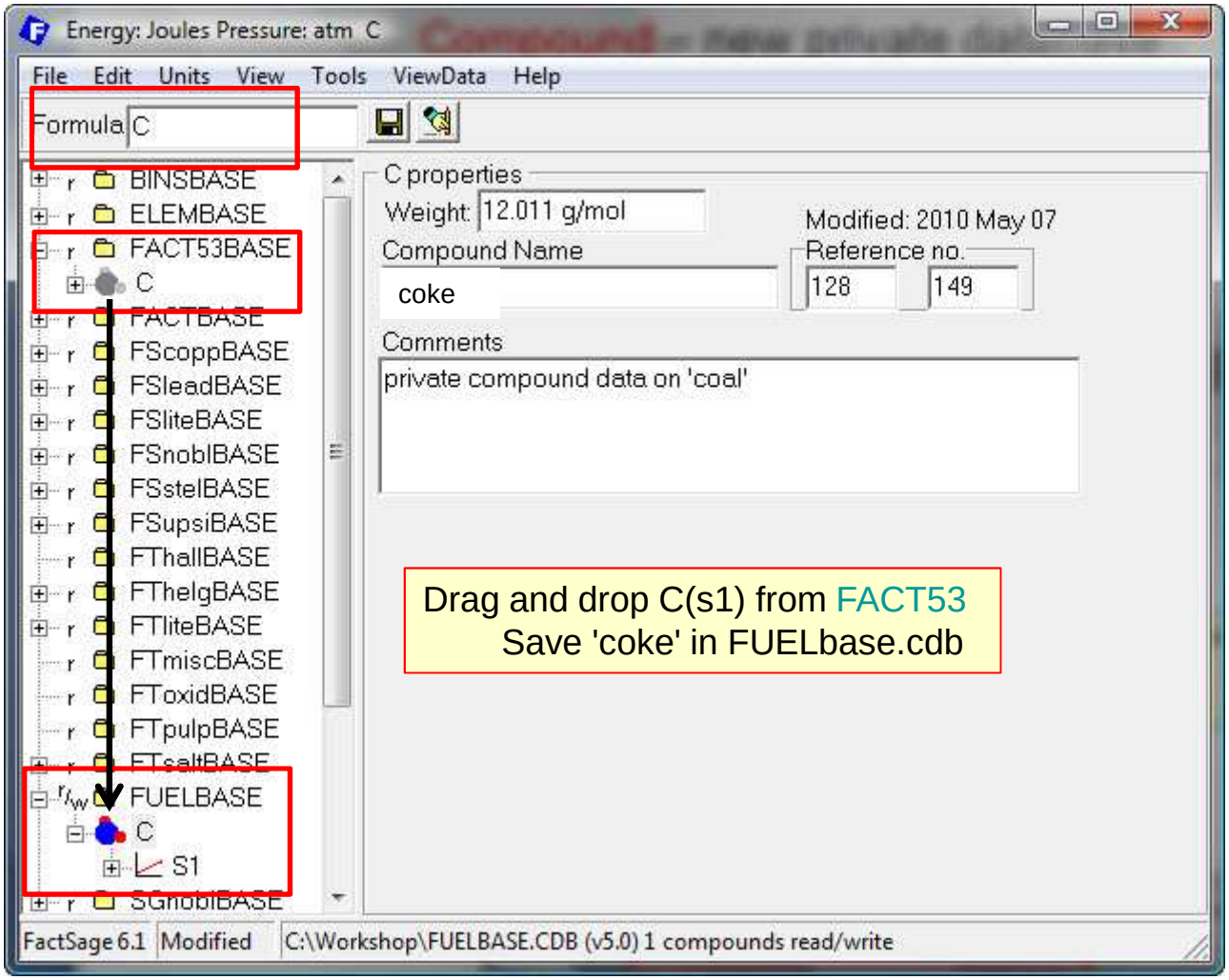
<A> = 0.90, Delta(H) = 0
=> Product T = 1956.59 °C

View Data
- non-ideal gas properties of **$H_2O(g)$**

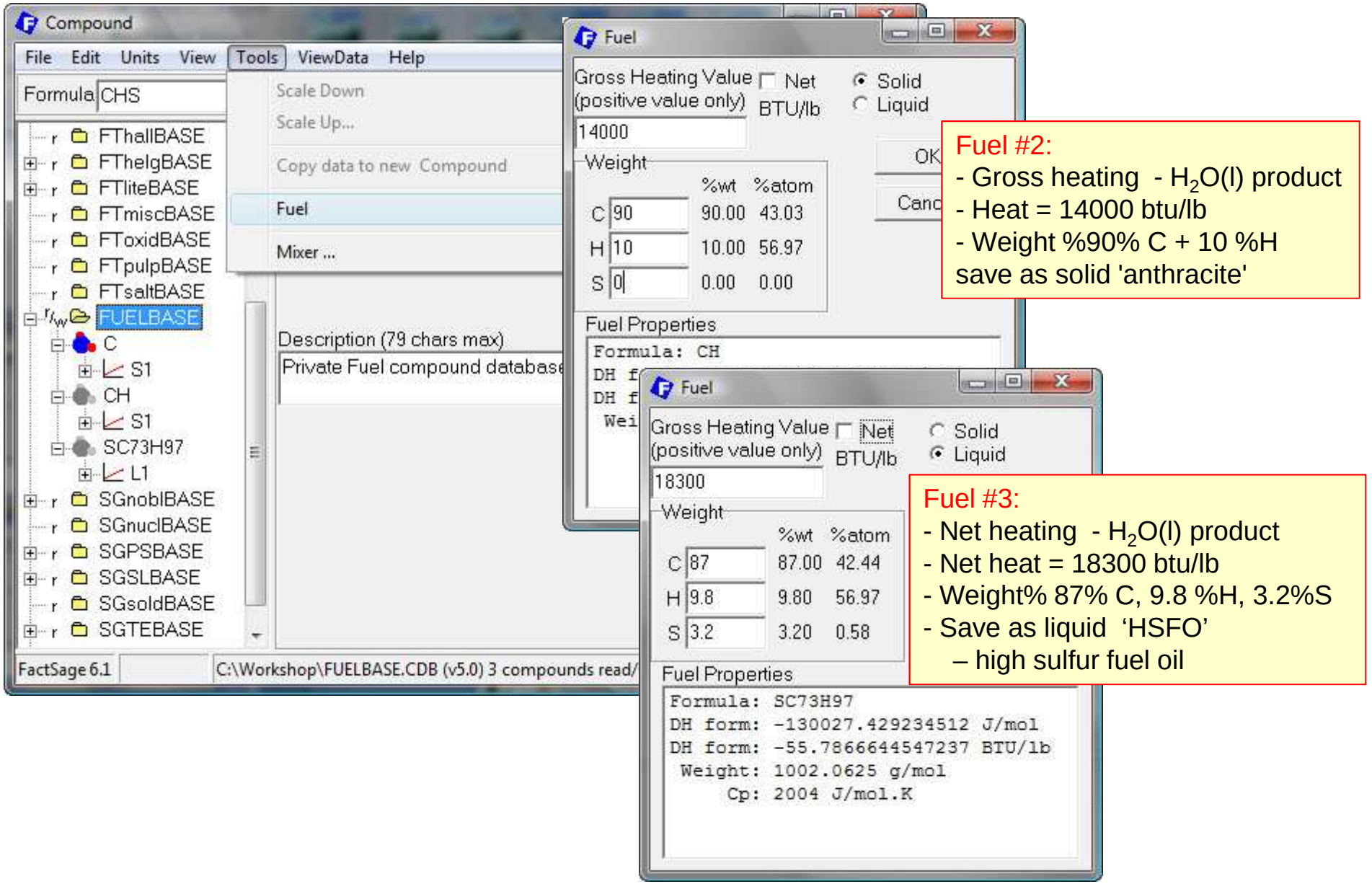
Compound – new private database



Compound – new private fuel data on ‘coke’



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

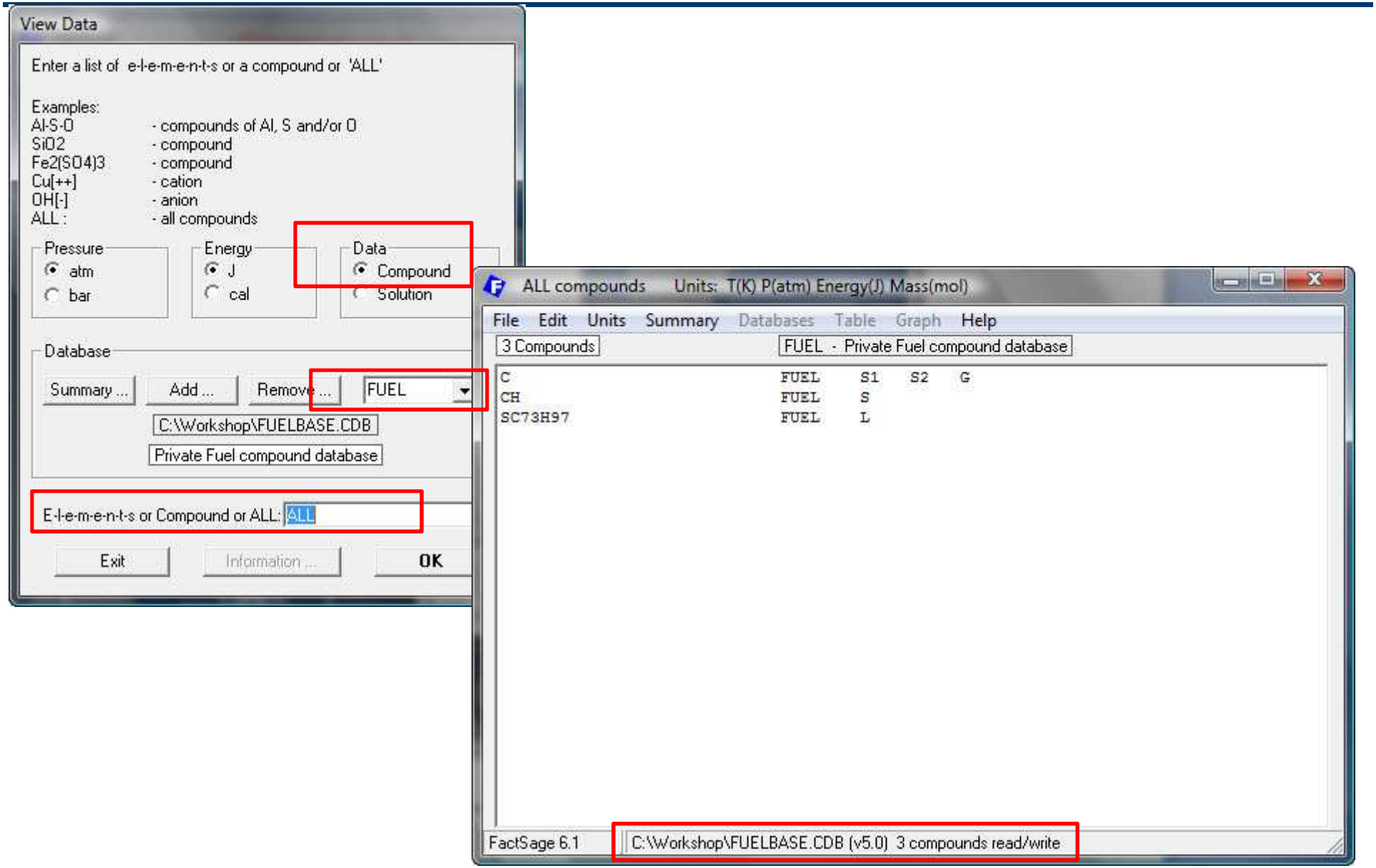


Fuel #2:
- Gross heating - H_2O(l) product
- Heat = 14000 btu/lb
- Weight %90% C + 10 %H

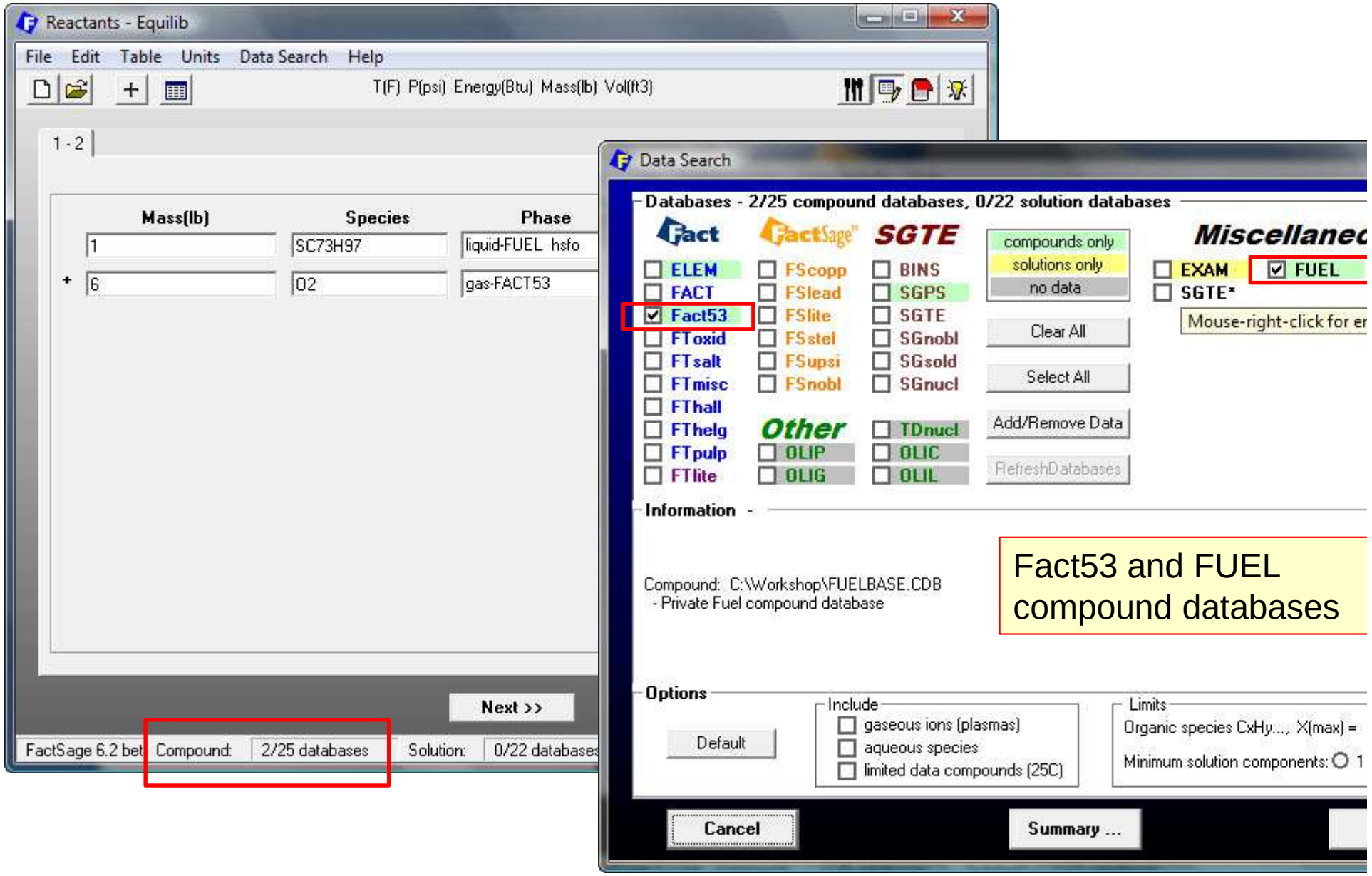
save as solid 'anthracite'

Fuel #3:
- Net heating - H_2O(l) product
- Net heat = 18300 btu/lb
- Weight% 87% C, 9.8 %H, 3.2%S
- Save as liquid ‘HSFO’
  - high sulfur fuel oil

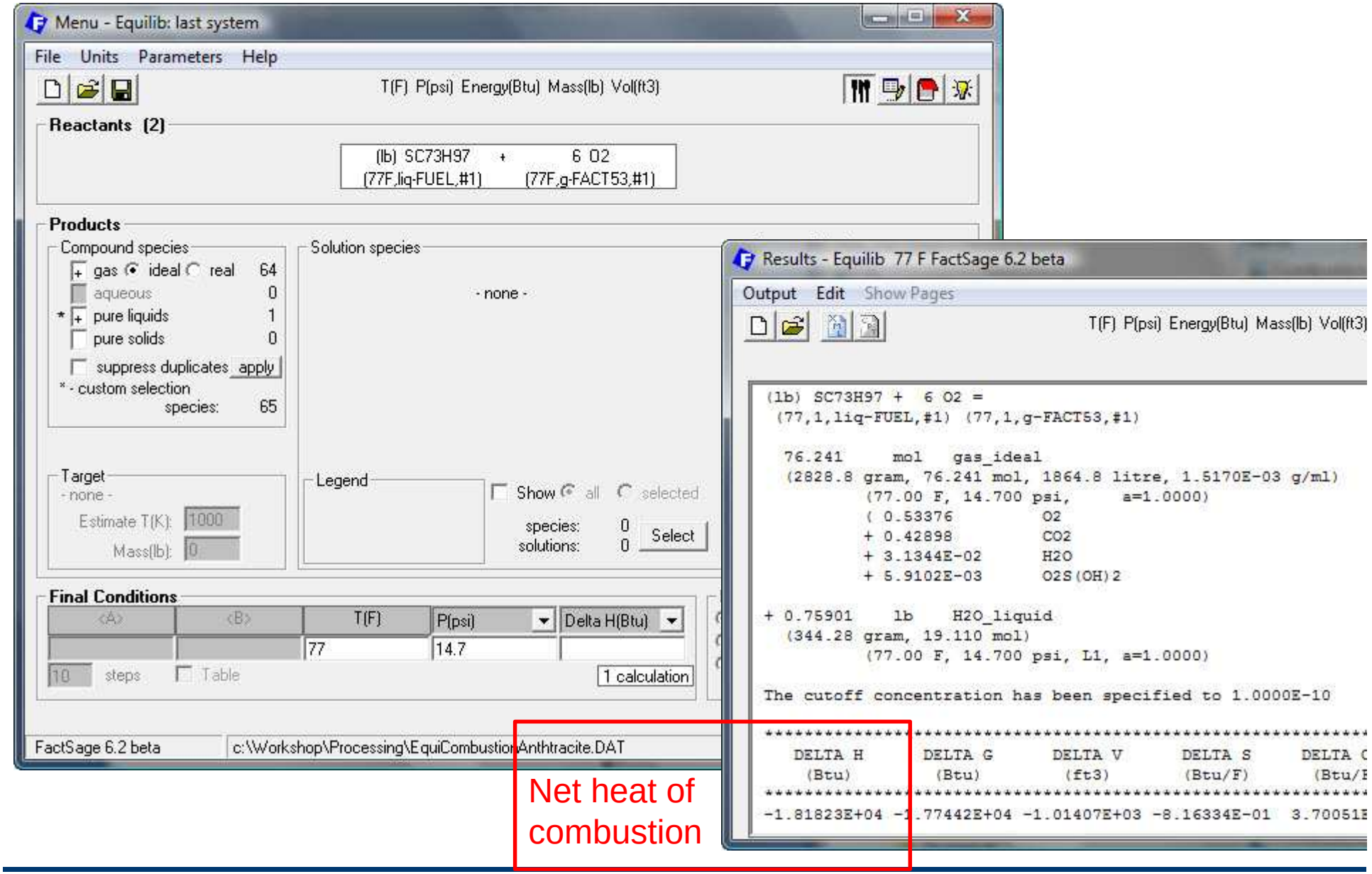
View Data – summary of FUEL compound data



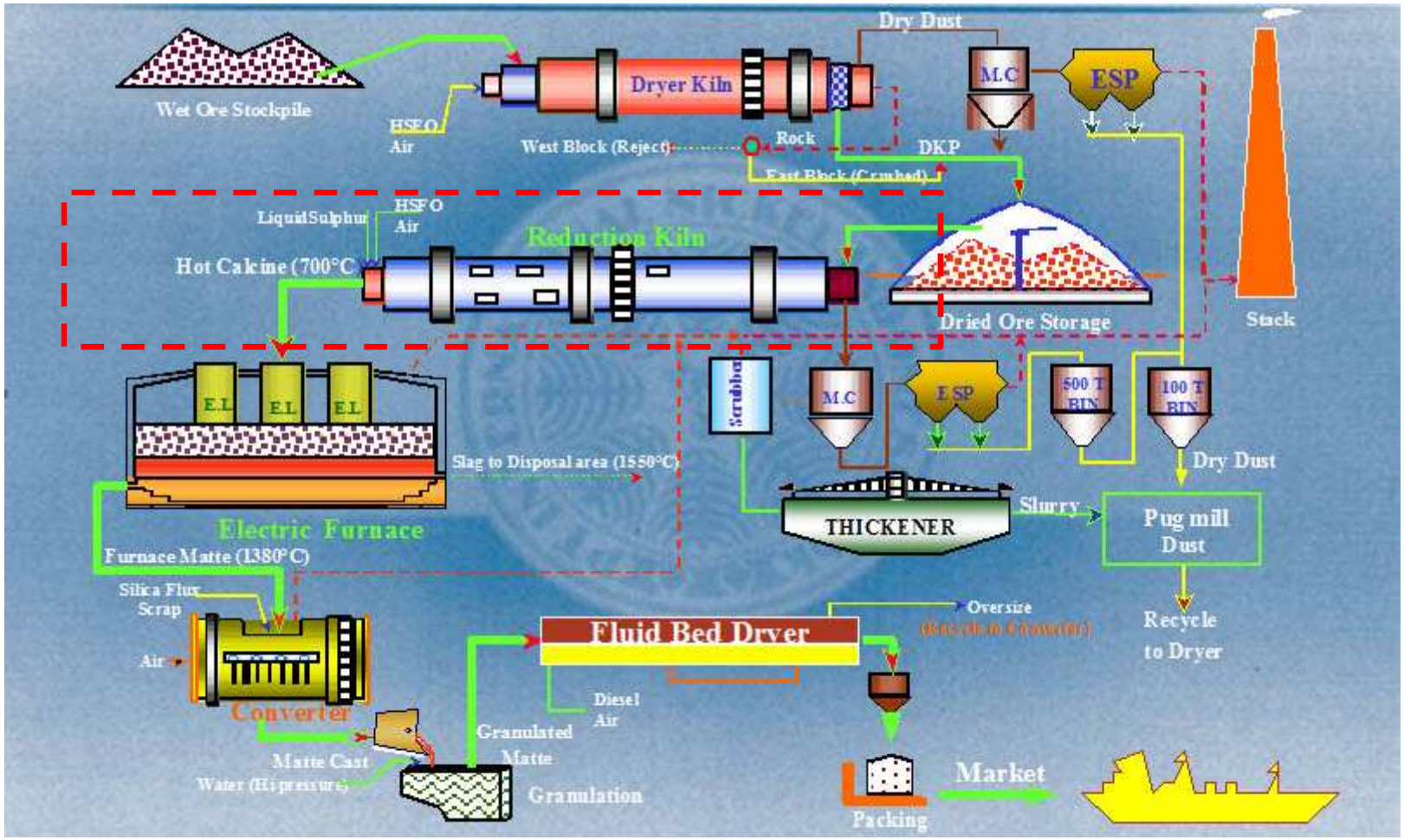
Equilib – combustion of HSFO 'high sulfur fuel oil'



Equilib – combustion of HSFO 'high sulfur fuel oil'



Databases – Reduction Kiln

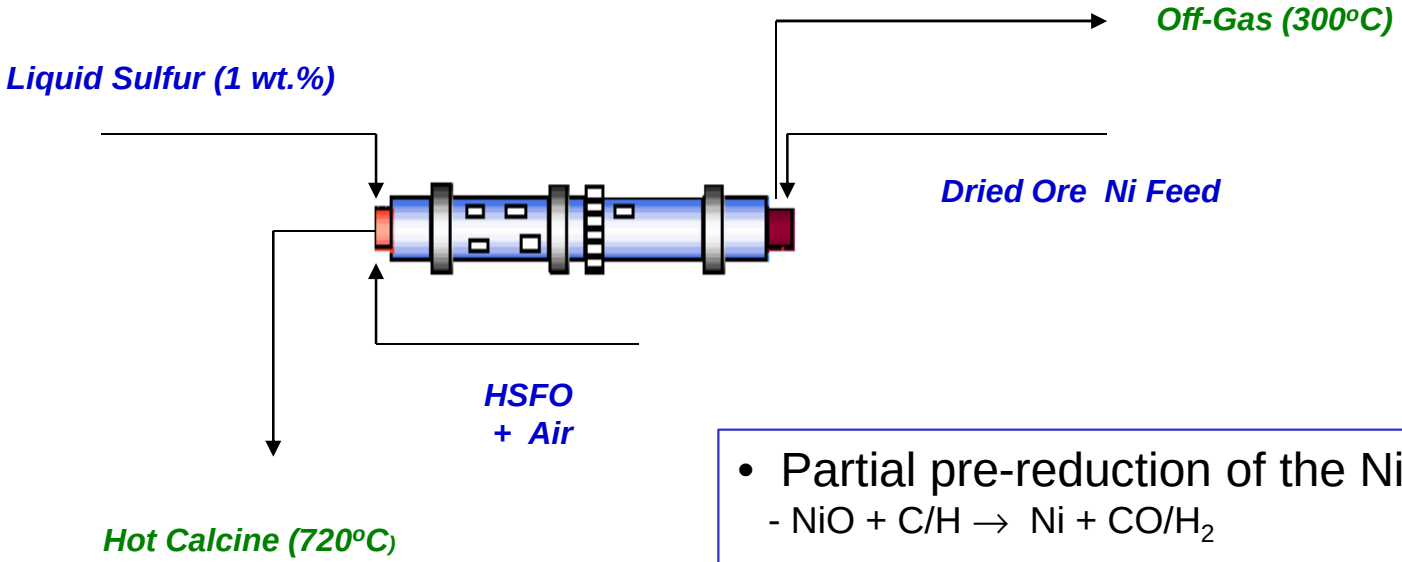


Databases

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

Equilib – Reduction kiln

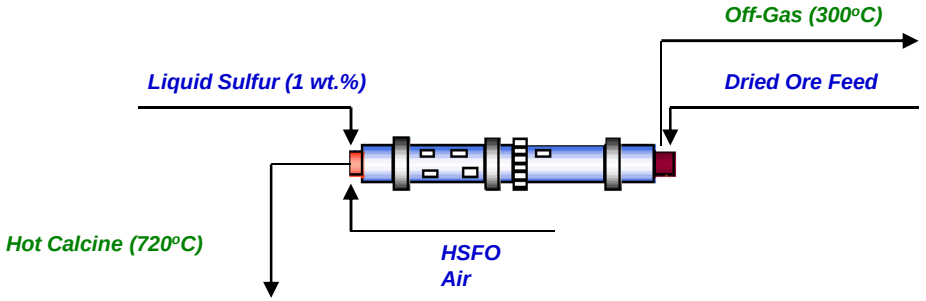
Reduction Kiln



- Partial pre-reduction of the Ni ore
  - $NiO + C/H \rightarrow Ni + CO/H_2$
- Sulfuration of the Ni
  - $NiO + C/H + S \rightarrow Ni_3S_2 + CO/H_2$
- Preheat the mineral
  - combustion of high sulfur fuel oil 'HSFO' => 720°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 SiO2 + 31 Fe2O3 + 2.672 NiO + 0.1 CoO + 1.5 C
Liquid Sulfur : + 1.0 S
HSFO + Air : + 4.6 C42H57S1 + 20.7 [Air_Real] =

100.48 litre Gas Ideal
(45.973 vol% N2
\+ 29.233 vol% CO
\+ 15.034 vol% *H2*
\+ *7.0830* *vol% CO2*
\+ *2.4305* *vol% H2O*
\+ *0.19281* *vol% CH4*
\+ 0.48174E-01 vol% H2S
\+ 0.29676E-02 vol% COS
\+ 0.24462E-02 vol% NH3)

\+ **3.2422 gram Beta_Ni2S** $(Fe_{0.30346}Ni_{0.37071}Va_{0.32583})_2S$

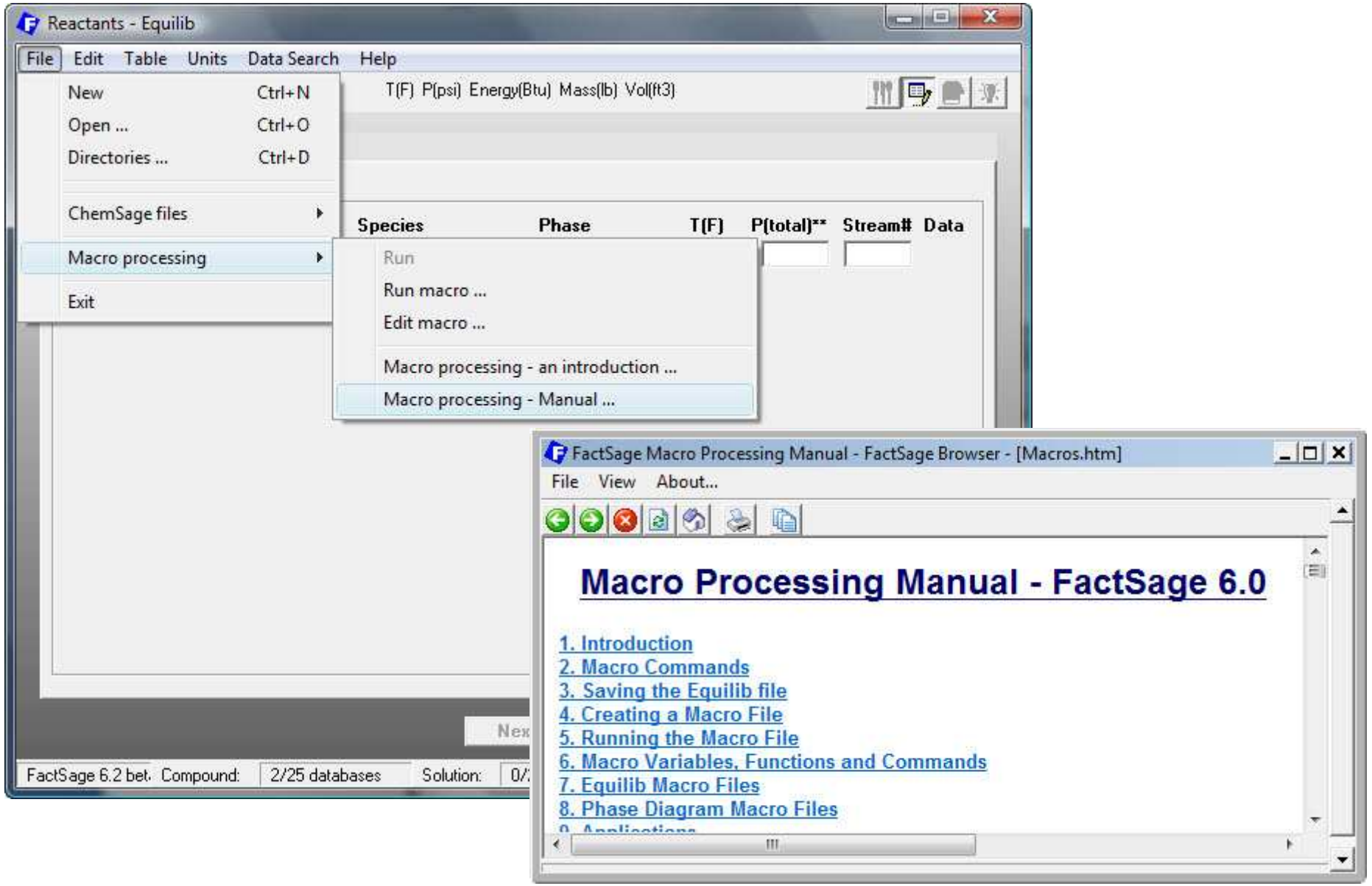
\+ **0.76615 gram Pyrrhotite** $(Fe_{0.86984}Ni_{7.6389E-2}Co_{5.2665E-2}Va_{1.1030E-3})S$

\+ **1.2169 gram FCC** **34.464 wt.% Fe + 62.184 wt.% Ni + 3.3517 wt.% Co**

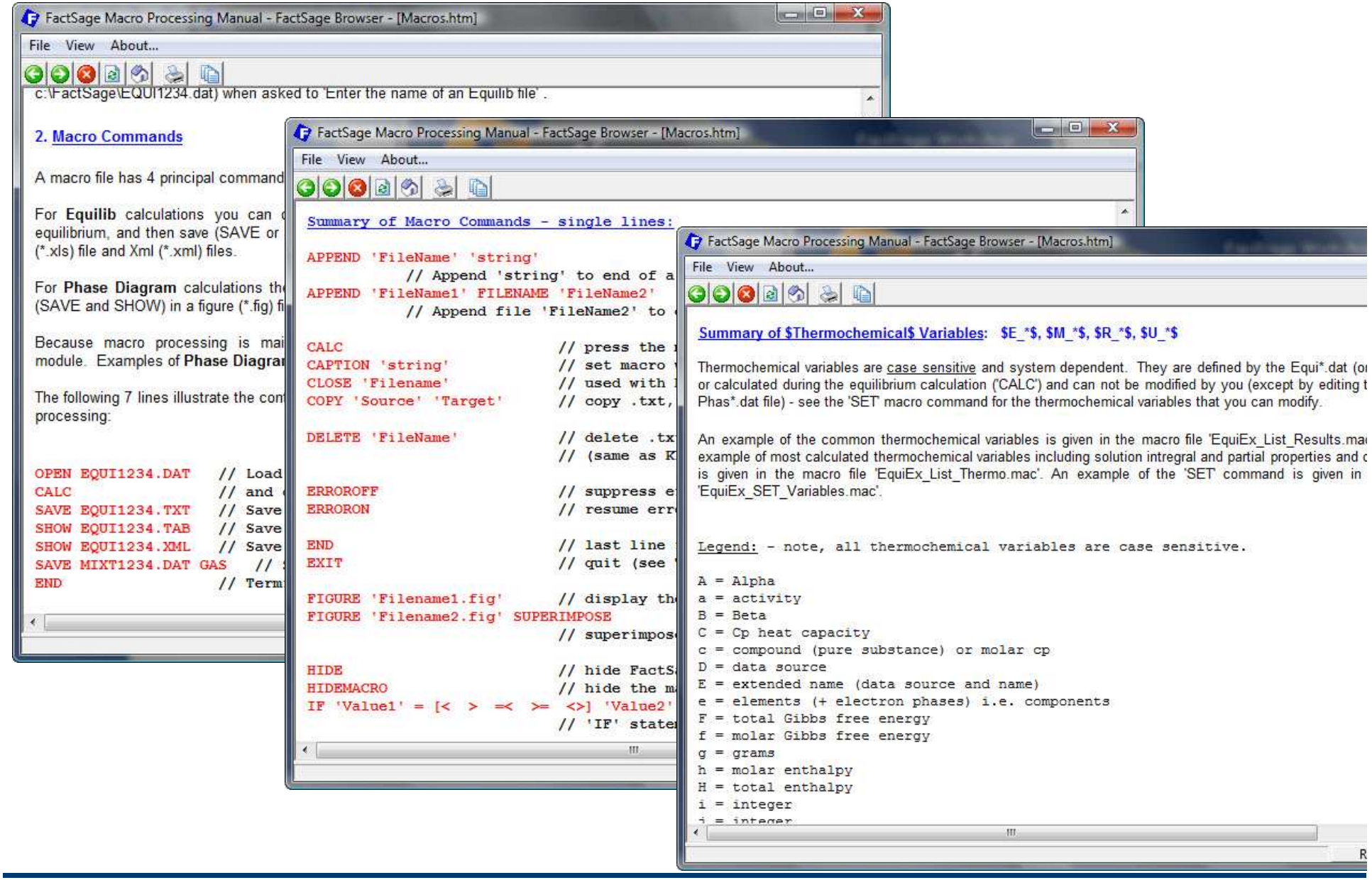
\+ **70.820 gram Orthopyroxene** $(Mg_{0.40234}Fe_{0.59766})\{Mg_{0.83571}Fe_{0.16394}Fe^{3+}_{3.5434E-4}\}[Fe^{3+}_{3.5434E-4}Si_{0.99965}]SiO_6$

\+ **22.735 gram Olivine** $(Mg_{0.55007}Fe_{0.4496}Co_{2.0573E-4}Ni_{1.2512E-4})\{Mg_{0.59855}Fe_{0.3985}Co_{1.1586E-3}Ni_{1.7900E-3}\}SiO_4$

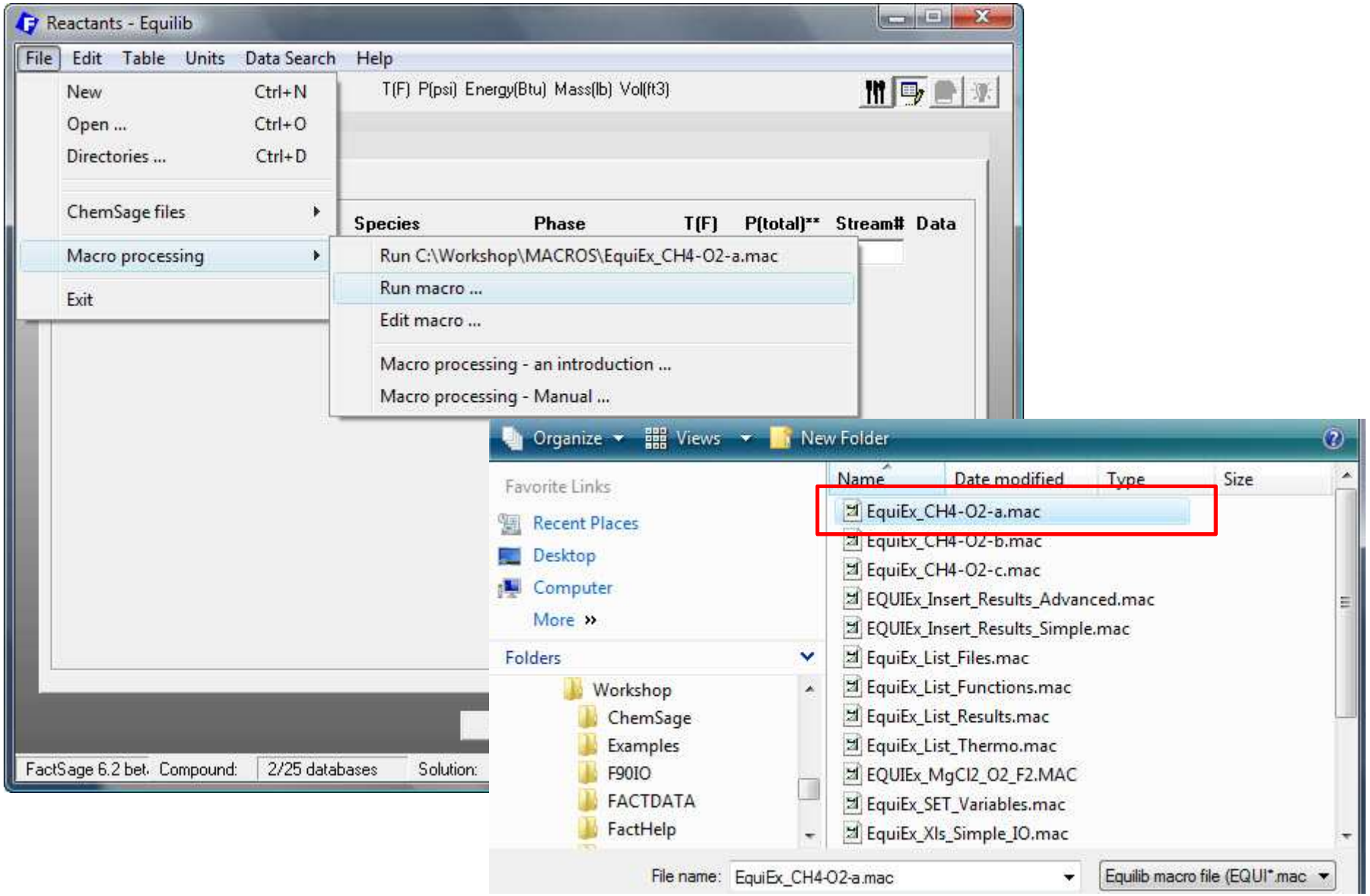
Equilib – Macro Processing



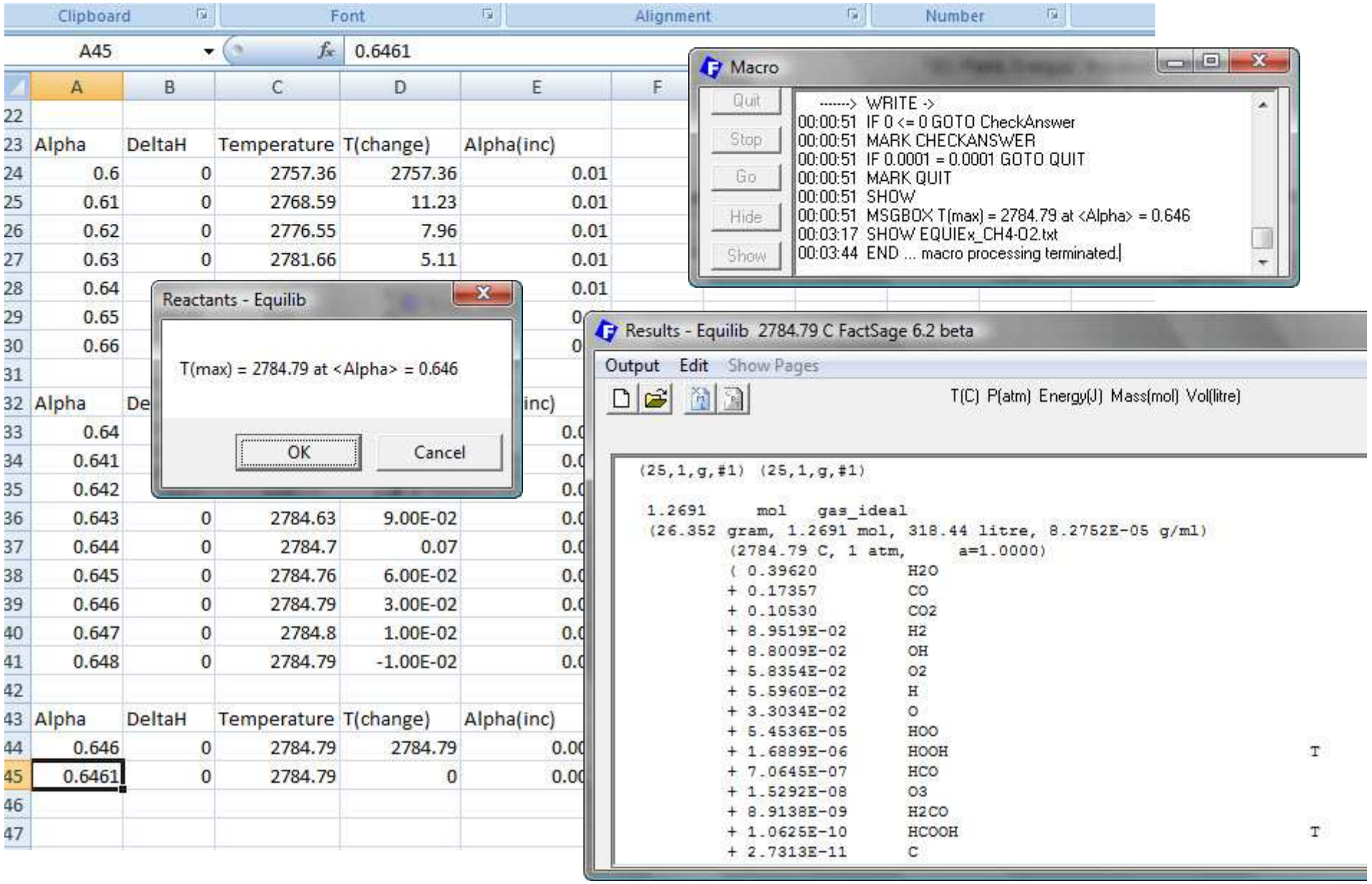
Macro Processing - Manual



Equilib – running a macro



Macro processing – Excel i/o : maximum flame temperature



Clipboard | Font | Alignment | Number

A45 | 0.6461

	A	B	C	D	E	F
22						
23	Alpha	DeltaH	Temperature	T(change)	Alpha(inc)	
24	0.6	0	2757.36	2757.36	0.01	
25	0.61	0	2768.59	11.23	0.01	
26	0.62	0	2776.55	7.96	0.01	
27	0.63	0	2781.66	5.11	0.01	
28	0.64				0.01	
29	0.65				0	
30	0.66				0	
31						
32	Alpha	De			inc)	
33	0.64				0.0	
34	0.641				0.0	
35	0.642				0.0	
36	0.643	0	2784.63	9.00E-02	0.0	
37	0.644	0	2784.7	0.07	0.0	
38	0.645	0	2784.76	6.00E-02	0.0	
39	0.646	0	2784.79	3.00E-02	0.0	
40	0.647	0	2784.8	1.00E-02	0.0	
41	0.648	0	2784.79	-1.00E-02	0.0	
42						
43	Alpha	DeltaH	Temperature	T(change)	Alpha(inc)	
44	0.646	0	2784.79	2784.79	0.00	
45	0.6461	0	2784.79	0	0.00	
46						
47						

Macro

Quit | Stop | Go | Hide | Show

```
------> 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 EQUIEx_CH4-O2.txt
00:03:44  END ... macro processing terminated.
```

Reactants - Equilib

T(max) = 2784.79 at <Alpha> = 0.646

OK | Cancel

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                              T
          + 7.0645E-07       HCO
          + 1.5292E-08       O3
          + 8.9138E-09       H2CO
          + 1.0625E-10       HCOOH                             T
          + 2.7313E-11       C
```