

The *Mixture* module

- Use *Mixture* to edit mixtures and streams for input to *Equilib*.
- NOTE that the use of the *Mixture* module is very closely linked with the *Equilib* module. Streams for example are generated in *Equilib* and the *Mixture* module is only used to edit them.

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The *Mixture* module



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

Creating and Saving *Mixture*

The following two slides show how a *Mixture* is created for use as a «combined» input in the *Equilib Reactants* screen.

Note that mixtures once created can also be edited/modified at a later time using the *Mixture* module.

Creating a *Mixture*

A mixture is a group of reactants that you normally enter via the *Equilib Reactants Window*.

The screenshot shows the 'Mixtures and Streams' window in FactSage 5.0. The window title is 'F Mixtures and Streams'. The menu bar includes 'File', 'Edit', 'Units', 'Data Search', and 'Mixture or Stream?'. Below the menu bar are icons for file operations and a '+' button. The main area displays a table with columns: 'Mass(mol)', 'Species', 'Phase', 'T(K)', and 'P(total)**'. The table contains four rows of data, all with a temperature of 298.15 K and a pressure of 1.0. The species are N2, O2, H2O, and CO2. The phases are 'gas', 'gas', 'gas steam', and 'gas'. The mass values are 0.79, 0.21, 0.01, and 350E-6 respectively. To the right of the table, the word 'FACT' is repeated for each row. Below the table, there is a 'total moles' field with the value 1.01035. The status bar at the bottom shows 'FactSage 5.0' and 'Compound: FACT EXAM ELEM SGPS SGSL Solution: FACT SGSL USER'.

Mass(mol)	Species	Phase	T(K)	P(total)**
0.79	N2	gas	298.15	1.0
+ 0.21	O2	gas	298.15	1.0
+ 0.01	H2O	gas steam	298.15	1.0
+ 350E-6	CO2	gas	298.15	1.0

total moles: 1.01035

Here in *Mixture*, you have entered 4 gaseous species.

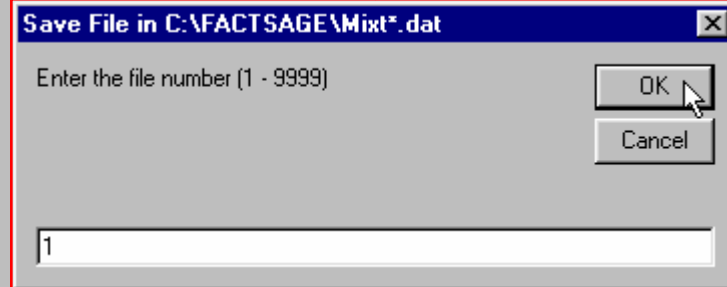
Total number of moles are automatically calculated by *Mixture*.

If you edit and change the «**total moles**» then the reactants moles will change correspondingly.

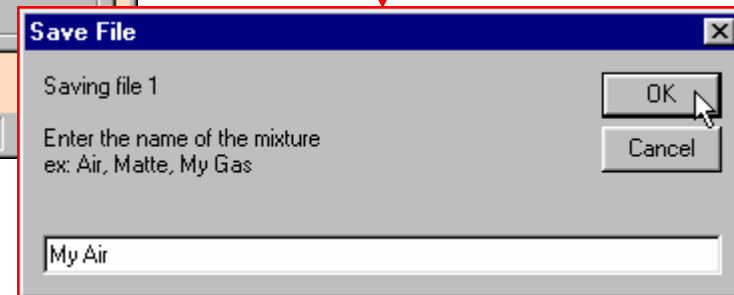
Saving the *Mixture*

Click on  to save your **mixture**.

Enter a file number: «**1**»



and a mixture name: «**My Air**».



Mixtures and Streams

File Edit Units Data Search Mixture or Stream?

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

1 - 4 Save

Mass(mol)	Species	Phase	T(K)	P(total)**
0.79	N2	gas	298.15	1.0
+ 0.21	O2	gas	298.15	1.0
+ 0.01	H2O	gas steam	298.15	1.0
+ 350E-6	CO2	gas	298.15	1.0

1.01035 total moles

FactSage 5.0 Compound: FACT EXAM ELEM SGPS SGSL Solution: FACT SGSL USER

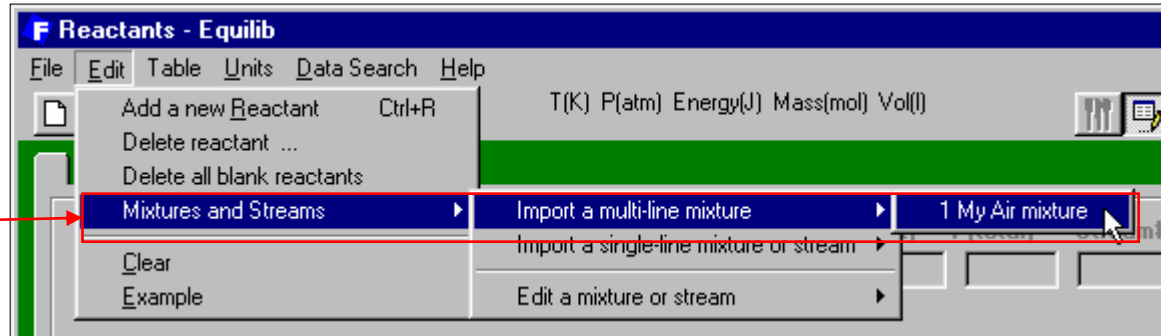
The mixture «My Air» generated with the Mixture module is imported into *Equilib* via the **Reactants screen**. Two possibilities are open: as a **single-line** input, i.e. similar to a pure substance, and as a **multi-line** input.

Furthermore it is possible to **manipulate the total amount** of a mixture before calculation begins.

The following three slides show how the above actions are performed.

Importing «My Air» into *Equilib* as a multi-line mixture

In the **Reactants** window of the *Equilib* program, select:
Edit > Mixtures and Streams > Import a multi-line mixture > 1 My Air mixture



The screenshot shows the 'Reactants - Equilib' window with a table of reactants. The table has columns for Mass(mol), Species, Phase, T(K), P(total)**, Stream#, and Data. The reactants are N2, O2, H2O, and CO2. A blue box highlights the table, and an arrow points from a text box below to the table.

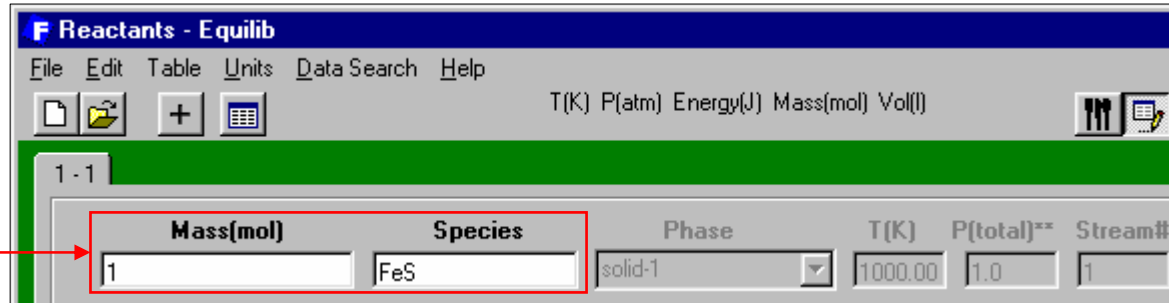
Mass(mol)	Species	Phase	T(K)	P(total)**	Stream#	Data
0.79	N2	gas	298.15	1	1	FACT
+ 0.21	O2	gas	298.15	1	1	FACT
+ 0.01	H2O	solid ice	298.15	1	1	FACT
+ 350E-6	CO2	gas	298.15	1	1	FACT

Importing as a multi-line mixture is equivalent to manually entering the reactants.

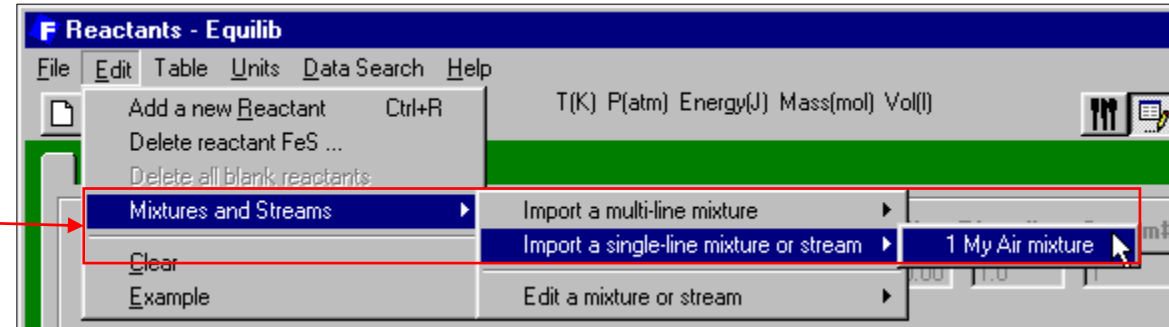
initial conditions

Importing «My Air» into *Equilib* as a **single-line** mixture

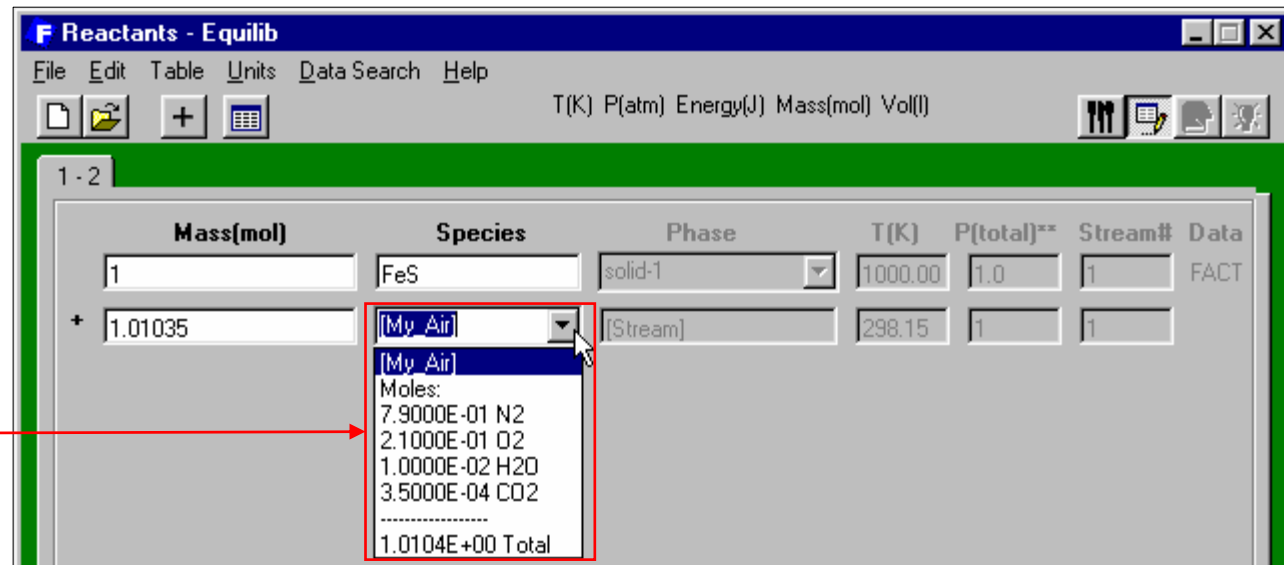
Let us say that you have already entered a reactant, **FeS**, in the **Reactants** window of the *Equilib* program.



To import a mixture, select: **Edit > Mixtures and Streams > Import a single-line mixture or stream > 1 My Air mixture**



Click on the down-arrow to get the list of **[My_Air]** mixture components.



Changing the **Mass input** of the mixture

Changing input to 1.0 mole.

The screenshot shows the 'Reactants - Equilib' window. A table lists reactants with columns for Mass(mol), Species, Phase, T(K), P(total)**, Stream#, and Data. The first row shows FeS with a mass of 1.0. The second row shows a mixture with a mass of 1.0. A dropdown menu is open for the second row, showing the composition of the mixture in moles.

Mass(mol)	Species	Phase	T(K)	P(total)**	Stream#	Data
1	FeS	solid-1	1000.00	1.0	1	FACT
+ 1.0	[My Air]	[Stream]	298.15	1	1	

Moles:
7.8191E-01 N2
2.0785E-01 O2
9.8976E-03 H2O
3.4641E-04 CO2

1.0000E+00 Total

The mixture automatically changes its composition.

Creating a **Stream**

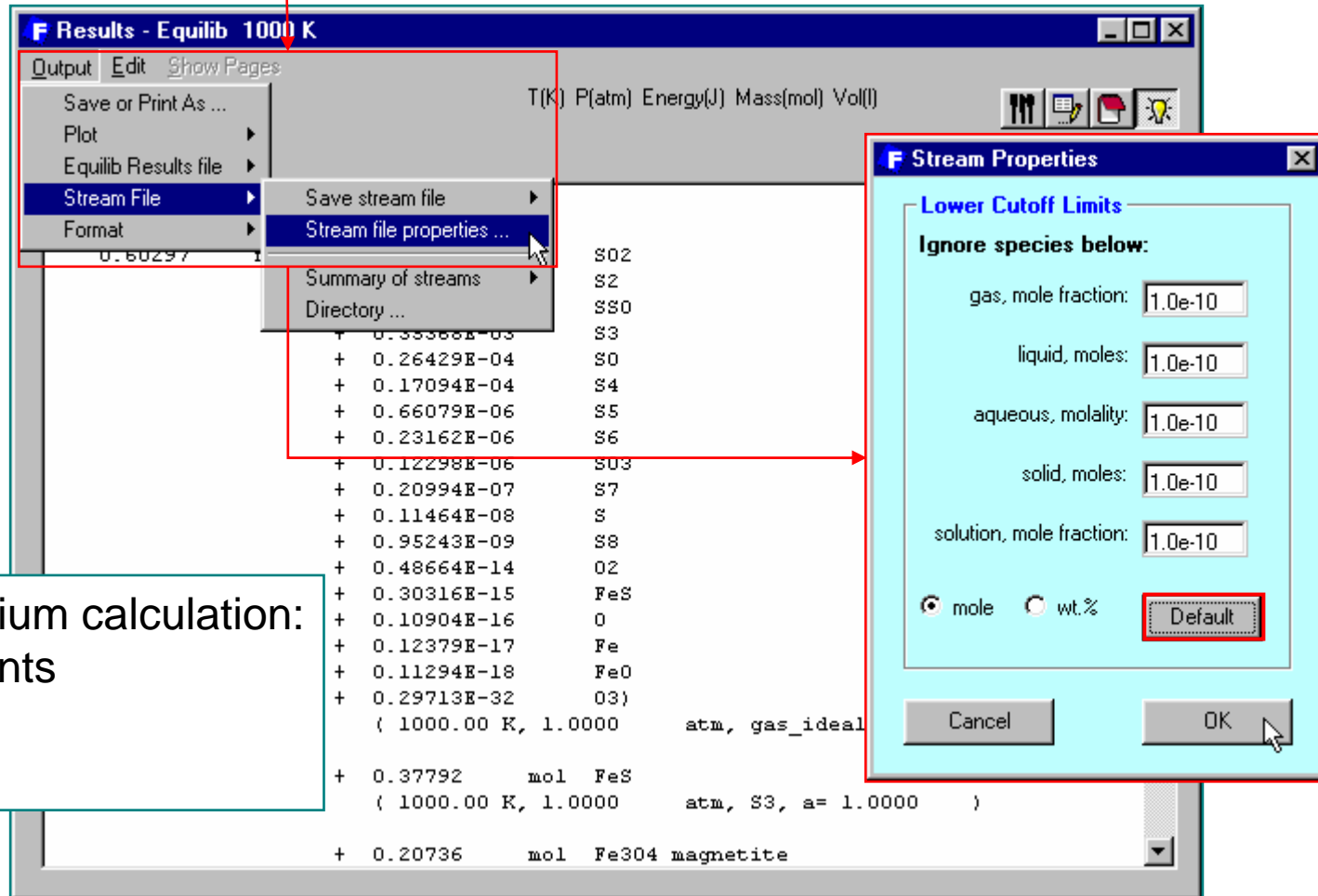
A **stream** is an equilibrated phase stored via the **Equilib Results** window. In other words, it contains a **set of amounts of the constituents** of a phase that was generated in an equilibrium calculation.

The following two slides show how **Equilib** is used to generate a **gas stream** from the **roasting** of FeS with O₂ (**FeS + O₂**, **T=1000K, P=1atm**).

Creating a **Stream** – Properties

A **stream** is an equilibrated phase stored via the **Equilib Results** window

Setting the cut-off limit for the stream species: **Output > Stream File > Stream file properties...** and selecting the **Default** values.



The screenshot shows the 'Equilib Results' window with the 'Stream File' menu open, highlighting 'Stream file properties...'. The 'Stream Properties' dialog box is open, showing 'Lower Cutoff Limits' for various species. The 'Default' button is selected. The 'Equilib Results' window shows a list of species and their amounts.

Species	Amount
S02	0.60297
S2	0.35368E-03
SS0	0.26429E-04
S3	0.17094E-04
S0	0.66079E-06
S4	0.23162E-06
S5	0.12298E-06
S6	0.20994E-07
S	0.11464E-08
S8	0.95243E-09
O2	0.48664E-14
FeS	0.30316E-15
O	0.10904E-16
Fe	0.12379E-17
Fe0	0.11294E-18
O3	0.29713E-32
atm, gas_ideal	(1000.00 K, 1.0000
mol FeS	+ 0.37792
atm, S3, a= 1.0000	(1000.00 K, 1.0000
mol Fe304 magnetite	+ 0.20736

Results of an equilibrium calculation:

- FeS + O₂ as reactants
- T = 1000 K
- P = 1 atm

Creating a **Stream** – Saving

The gas phase contains the oxidation products of FeS + O₂ roasting at 1000 K

Creating a gas stream: Output > Stream File > Save stream file > Save gas phase...

The screenshot shows the 'Results - Equilib 1000 K' window. The 'Stream File' menu is open, and 'Save gas phase ...' is selected. The window displays a table of results with columns for T(K), P(atm), Energy(J), Mass(mol), and Vol(l). The table lists various species and their amounts, including S0, S4, S5, S6, S03, S7, S, S8, O2, FeS, O, Fe, Fe0, O3, and Fe304 magnetite.

T(K)	P(atm)	Energy(J)	Mass(mol)	Vol(l)
0.35368E-03				
+ 0.26429E-04	S0			
+ 0.17094E-04	S4			
+ 0.66079E-06	S5			
+ 0.23162E-06	S6			
+ 0.12298E-06	S03			
+ 0.20994E-07	S7			
+ 0.11464E-08	S			
+ 0.95243E-09	S8			
+ 0.48664E-14	O2			
+ 0.30316E-15	FeS			
+ 0.10904E-16	O			
+ 0.12379E-17	Fe			
+ 0.11294E-18	Fe0			
+ 0.29713E-32	O3)			
(1000.00 K, 1.0000	atm, gas_ideal)			
+ 0.37792	mol FeS			
(1000.00 K, 1.0000	atm, S3, a= 1.0000			
+ 0.20736	mol Fe304 magnetite			

Enter a file number: «**2**»

The dialog box is titled 'Save File in C:\FACTSAGE\Mixt*.dat'. It contains the text 'Enter the stream file number (1 - 9999)' and a text input field containing the number '2'. There are 'OK' and 'Cancel' buttons.

and a stream name: «**Roaster Gas**».

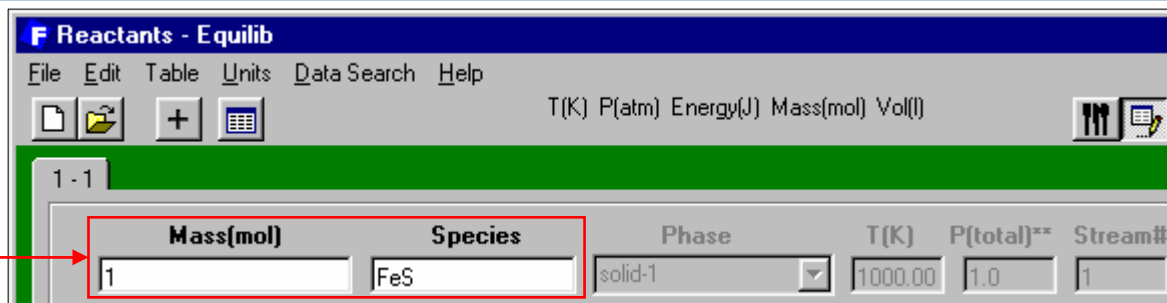
The dialog box is titled 'Save File'. It contains the text 'Saving file 2' and 'Enter the name of the stream ex: Roaster Gas, Cu Matte, Slag'. A text input field contains the name 'Roaster Gas'. There are 'OK' and 'Cancel' buttons.

The stream «Roaster Gas» generated from Equilib output (see above) is used as a **single-line input**. The initial **amount** (as calculated) is **modified** before calculation takes place.

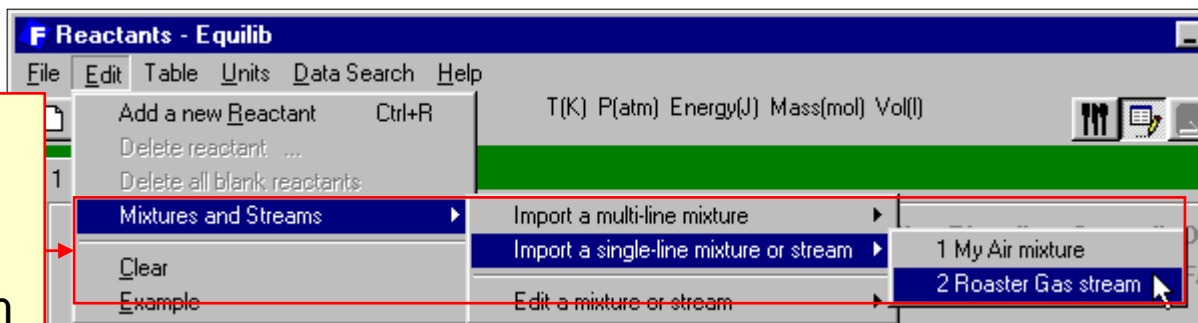
All of these **actions** take place in the **Reactants screen** of the *Equilib* module.

Importing «Roaster Gas» into *Equilib* as a **single-line** mixture

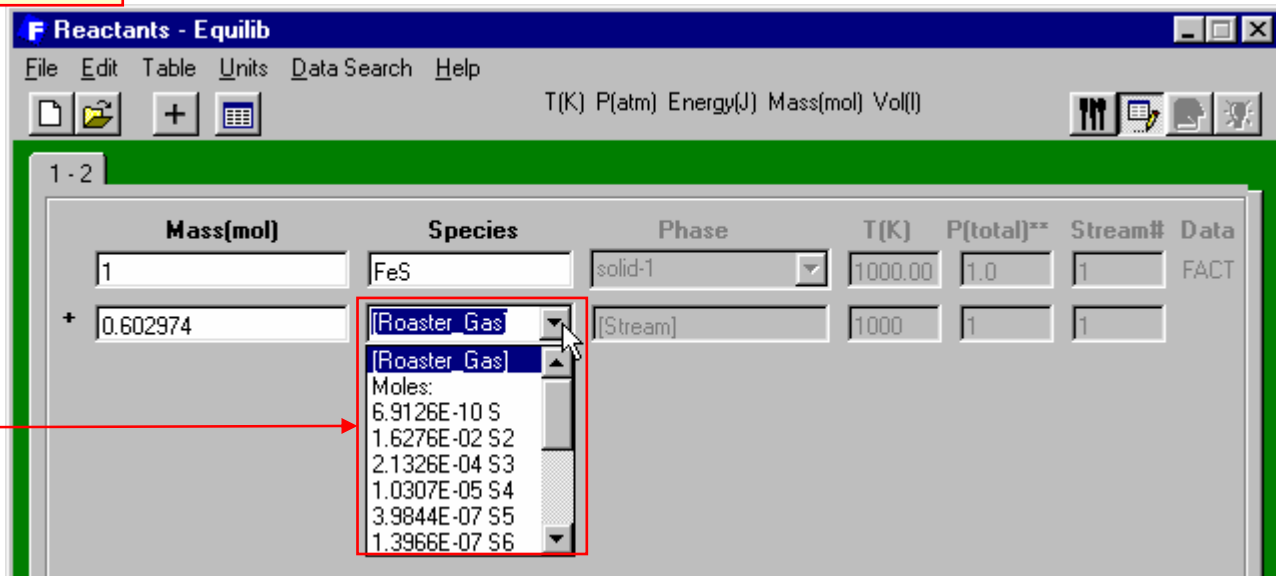
Let us say that you have already entered a reactant, **FeS**, in the **Reactants** window of the *Equilib* program.



To import a mixture, select: **E**dit > **M**ixtures and Streams > **I**mport a single-line mixture or stream > **2 Roaster Gas** stream



Click on the down-arrow to get the list of **[Roaster_Gas]** stream components.



Changing the **Mass input** of the stream

Changing input to 0.5 mole.

The screenshot shows the 'Reactants - Equilib' window in FactSage 5.0. The main table has the following data:

Mass(mol)	Species	Phase	T(K)	P(total)**	Stream#	Data
1	FeS	solid-1	1000.00	1.0	1	FACT
+ 0.5	[Roaster Gas]	[Stream]	1000	1	1	

The dropdown menu for the second row is open, showing the following options:

- [Roaster Gas]
- [Roaster Gas]
- Moles:
- 5.7321E-10 S
- 1.3496E-02 S2
- 1.7684E-04 S3
- 8.5471E-06 S4
- 3.3039E-07 S5
- 1.1581E-07 S6

The 'Next >>' button is visible at the bottom of the table area. The status bar at the bottom shows 'FactSage 5.0' and 'Compound: FACT EXAM ELEM SGPS SGSL Solution: FACT SGSL USER'.

The stream automatically changes its composition.

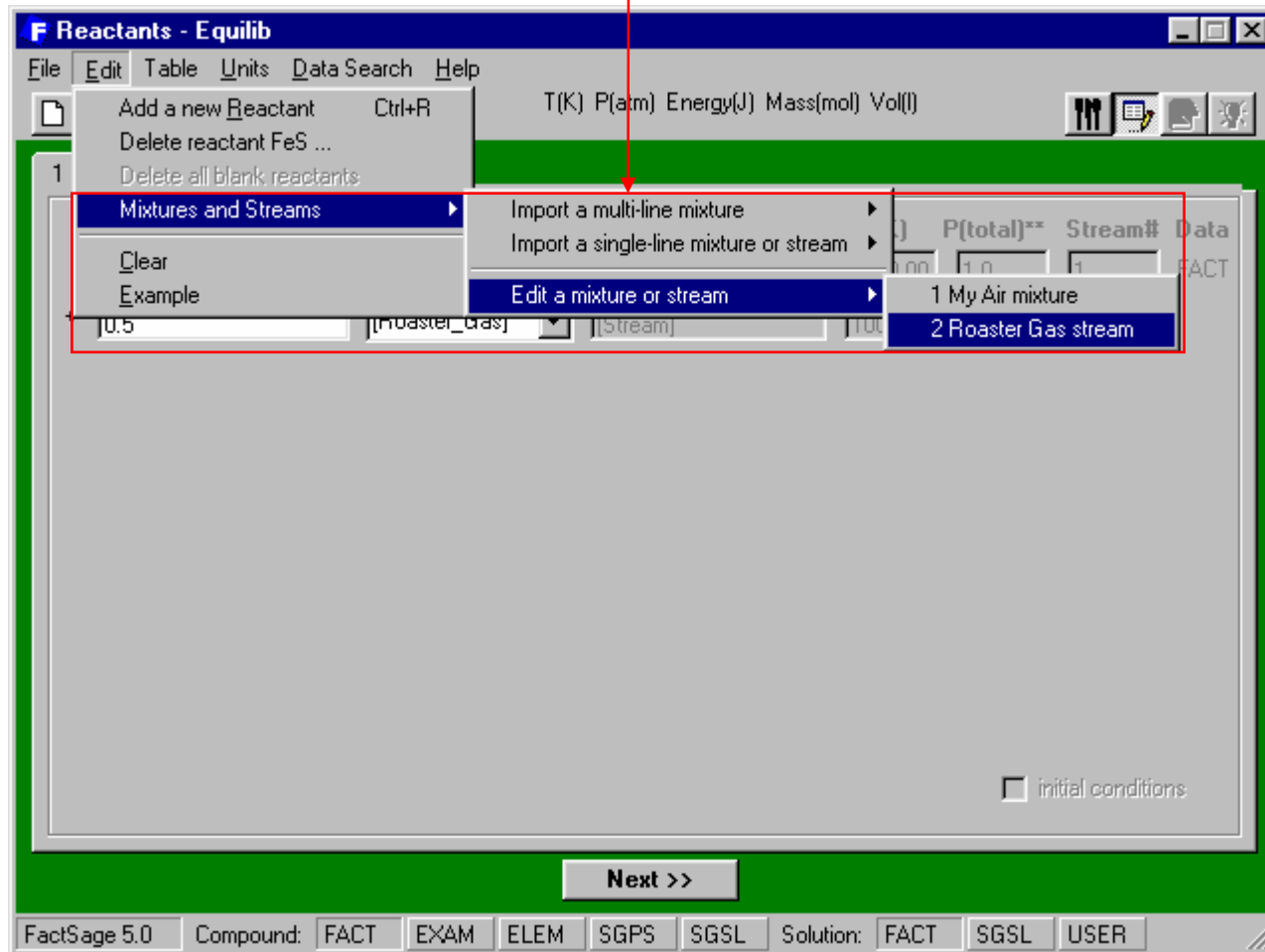
Editing a single-line mixture (or stream)

When in the **Reactants screen** of the **Equilib** module it is not only possible to import stored mixtures or stream, there is also an option to enter directly into the **Mixture** module for **editing** the chosen **mixture or stream**.

The following three slides show **how to do** this.

Opening a single-line mixture (or stream) for purposes of **editing**

To edit a mixture or a stream, select: **E**dit > Mixtures and Streams > Edit a mixture or stream > 2 **R**oaster **G**as stream



Editing a single-line mixture (or stream) in the *Mixture* program

Reactants - Equilib

File Edit Table Units Data Search Help

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

1 - 2

Mass(mol)	Species	Phase	T(K)	P(total)**	Stream#	Data
1	FeS	solid-1	1000.00	1.0	1	FACT
+ 0.5	[Roaster_Gas]	[Stream]	10			

- editing a mixture -

Next >>

FactSage 5.0 Compound: FACT EXAM ELEM SGPS SGSL Solution:

Mixtures and Streams

File Edit Table Units Data Search Mixture or Stream?

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

Row	Mass(mol)	Species
1	6.91259000000000000000E-10	S
2	1.62758700000000000000E-02	S2
3	2.13259800000000000000E-04	S3
4	1.03073600000000000000E-05	S4
5	3.98438700000000000000E-07	S5
6	1.39662800000000000000E-07	S6
7	1.26590000000000000000E-08	S7
8	5.74293400000000000000E-10	S8
9	1.59361400000000000000E-05	S0
10	5.84092200000000000000E-01	S02
11	7.41555100000000000000E-08	S03
12	2.36573700000000000000E-03	S00

12 species total moles

FactSage

Changing input to 0.5 mole.

Editing a single-line mixture (or stream) in the *Mixture* program

The stream automatically changes.

You can save your modifications

The screenshot shows the 'Mixtures and Streams' window in FactSage. The menu bar includes File, Edit, Table, Units, Data Search, and Mixture or Stream?. The toolbar contains icons for file operations and a 'Save' button. A table titled 'Stream Species' is displayed with 12 rows. Below the table, there is a label '12 species' and a text input field containing '0.5', followed by the text 'total moles'. The FactSage logo is visible in the bottom left corner.

Row	Mass(mol)	Species
1	5.7320806E-10	S
2	1.3496330E-02	S2
3	1.7683999E-04	S3
4	8.5471030E-06	S4
5	3.3039465E-07	S5
6	1.1581165E-07	S6
7	1.0497138E-08	S7
8	4.7621746E-10	S8
9	1.3214618E-05	S0
10	0.4843429	S02
11	6.1491476E-08	S03
12	1.9617242E-03	SS0