

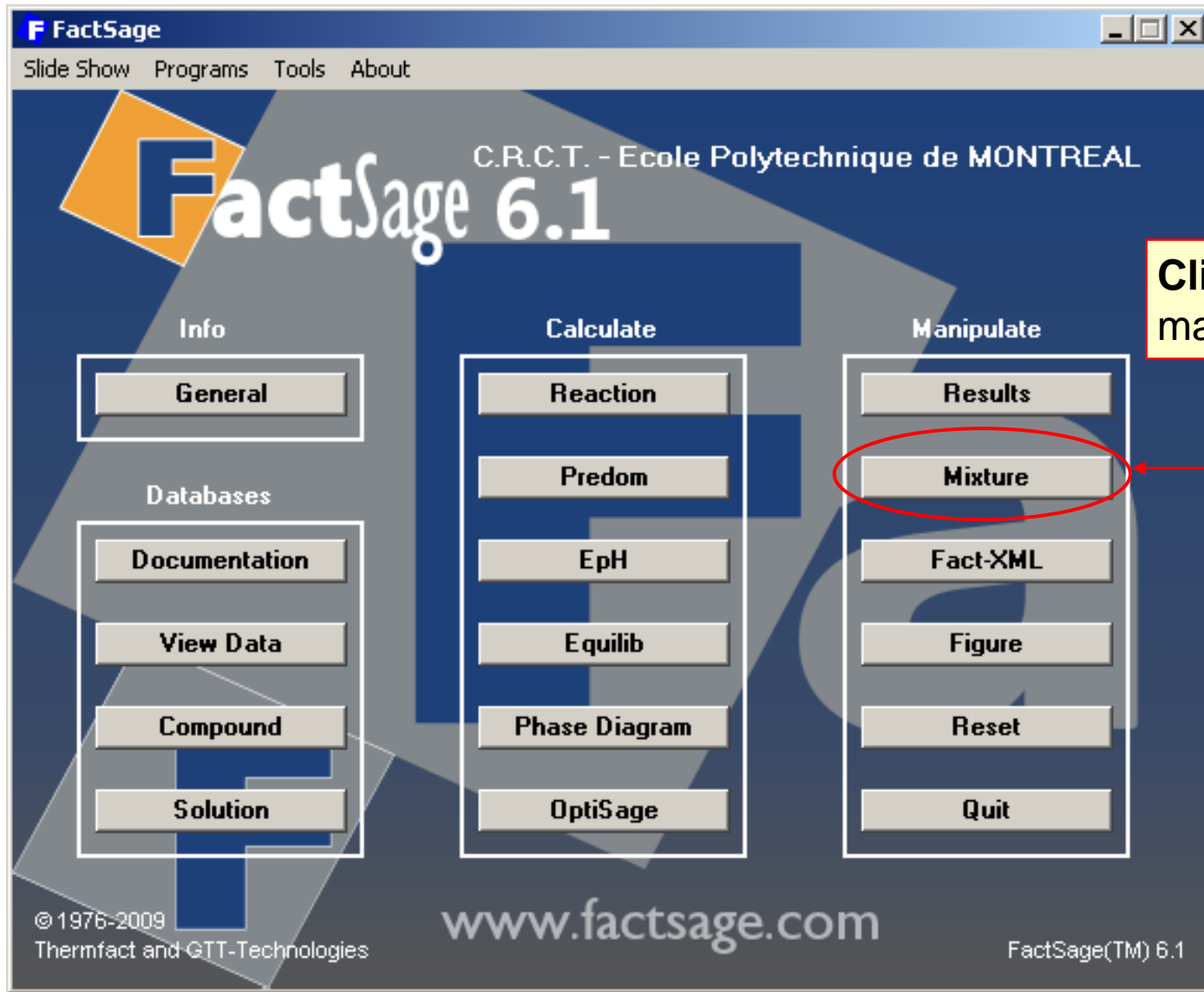
The *Mixture* module

- 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.

Table of contents

Section 1	<u>Table of contents</u>
Section 2	<u>Open the <i>Mixture</i> module</u>
Section 3	<u>Creating and Saving a <i>Mixture</i></u>
Section 4	<u>Importing «My Air» into <i>Equilib</i> and manipulating the total amount</u>
Section 5	<u>Creating a Stream</u>
Section 6	<u>Importing «Roaster Gas» into <i>Equilib</i> as a single-line mixture and manipulating its amount</u>
Section 7	<u>Editing a single-line mixture (or stream)</u>

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*.

Click on «**Units**» to change the settings. Here we are using T(K), P(atm), Energy (J) and Mass(mol).

The screenshot shows the 'Mixture and Streams' window in FactSage. The 'Units' menu is highlighted, showing settings for T(K), P(atm), Energy(J), Mass(mol), and Vol(litre). A table lists four reactants: N2, O2, H2O, and CO2, all at 298.15 K and 1.0 atm. The total moles are calculated as 1.01035.

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

Here in *Mixture*, we have entered 4 gaseous species at 298.15 K.

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**»

Save File in c:\FactSage\Mixt*.dat

Enter a stream file number
(1 - 9999)

or enter a stream file name (up to 26 characters), for
example

My very favorite stream

- avoid the special characters ?@/!"~`"'%&%+;<>{} \

1

and a mixture name: «**My Air**».

Save File c:\FactSage\Mixt1.DAT

Saving file 1

Enter the name of the mixture (upto 26 characters)
ex: Air, Matte, My Gas

My Air

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

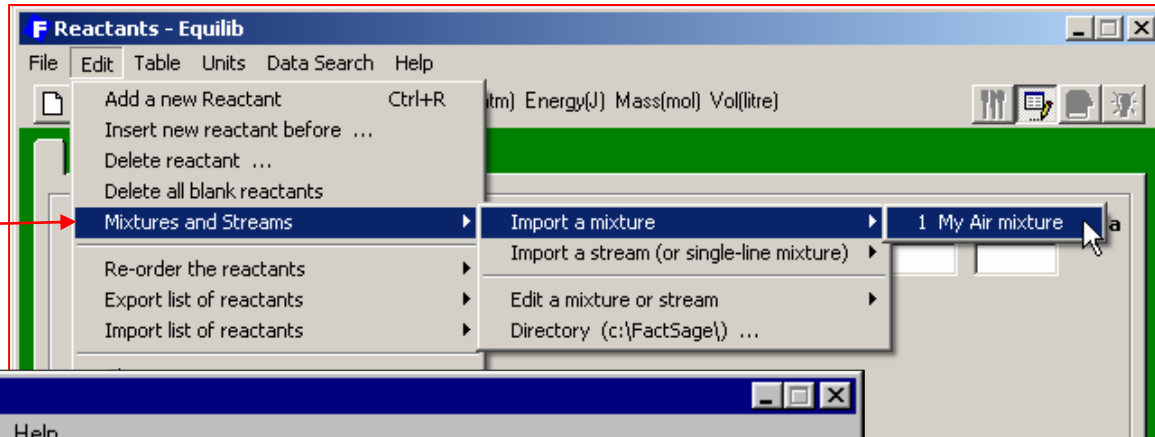
The mixture «My Air» generated with the Mixture module is imported into *Equilib* via the **Reactants screen**. Two possibilities are open: as a **single-line** input, i.e. similar to a pure substance, and as a **multi-line** input.

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, all at T=298.15 K and P=1. The H2O phase is set to 'solid ice'. A blue arrow points from the 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

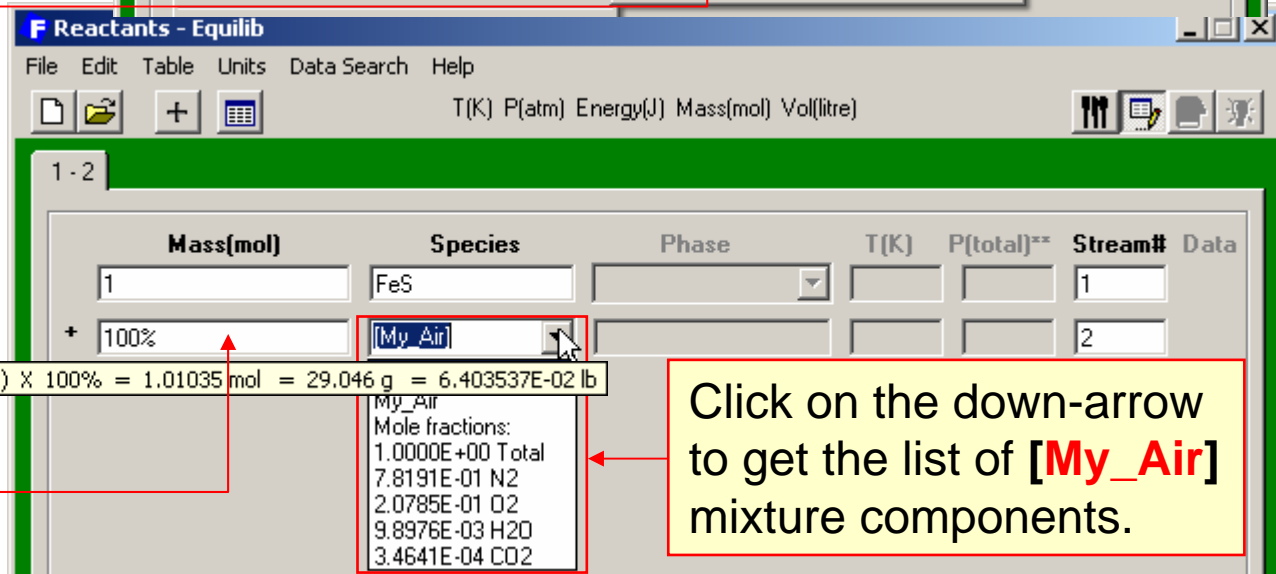
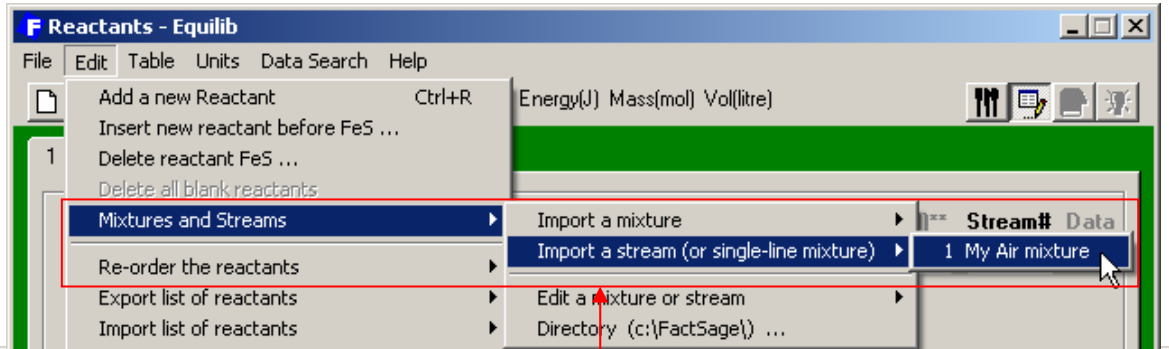
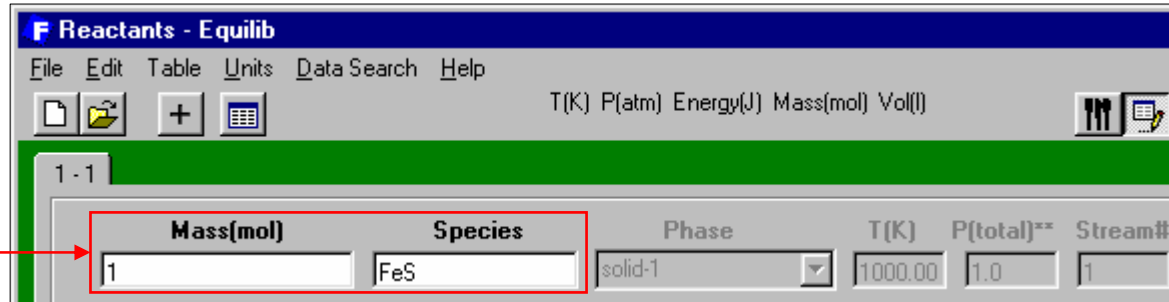
Importing as a multi-line mixture is equivalent to manually entering the reactants.

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: **E**dit > **M**ixtures and **S**treams > **I**mport a single-line mixture or stream > **1 My Air** mixture



Point cursor to display details on the Mass.

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.

Reactants - Equilib

File Edit Table Units Data Search Help

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

Mass(mol)	Species	Phase	T(K)	P(total)**	Stream#	Data
1	FeS				1	
+ 1	[My_Air]				2	

Initial Conditions

Next >>

FactSage Compound: 1/28 databases Solution: 1/23 databases

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 for a calculation at 1000 K. The 'Stream File' menu is open, and 'Stream file properties...' is selected. The 'Stream Properties' dialog box is open, showing 'Lower Cutoff Limits' for various species. The 'mole' radio button is selected, and the 'Default' button is highlighted. The 'Equilib Results' window shows a list of species and their amounts, with 'FeS_solid' highlighted at the bottom.

Species	Amount
SS0	3.9234E-03
S3	3.5368E-04
S0	2.6429E-05
S4	1.7094E-05
S5	6.6079E-07
S6	2.3162E-07
S03	1.2298E-07
S7	2.0994E-08
S	0.37792 mol
S8	
O2	
FeS	
O	
Fe	
FeO	
O3	

FeS_solid (33.224 gram, 0.37792 mol)

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 FactSage Mixture 5.2 interface. The main window displays the 'Output' menu with 'Stream File' > 'Save stream file' > 'Save gas phase...' selected. A dialog box prompts for a file number '2'. Another dialog box prompts for a stream name 'Roaster Gas'.

Enter a file number: «2»

and a stream name: «Roaster Gas».

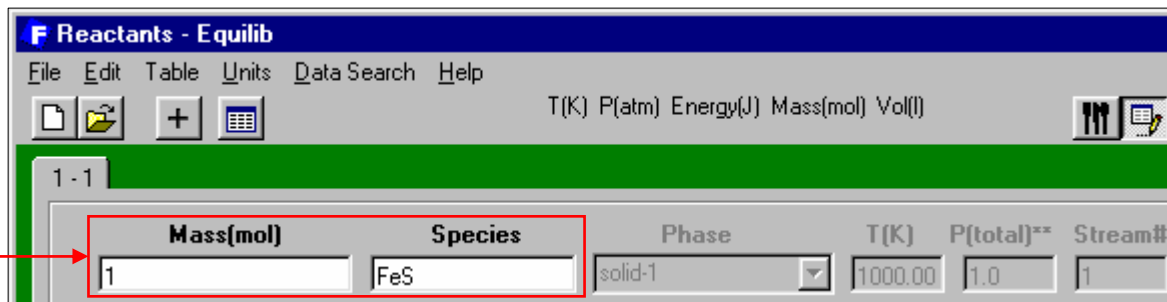
	T(K)	P(atm)	Energy(J)	Mass(mol)	Vol(litre)
+ 2.6					
+ 3.9234E-03				SS0	
+ 3.5368E-04				S3	
+ 2.6429E-05				S0	
+ 1.7094E-05				S4	
+ 6.6079E-07				S5	
+ 2.3162E-07				S6	
+ 1.2298E-07				S03	
+ 2.0994E-08				S7	
+ 1.1464E-09				S	
+ 9.5243E-10				S8	
+ 4.8664E-15				O2	
+ 3.0316E-16				FeS	
+ 1.0904E-17				O	
+ 1.2379E-18				Fe	
+ 1.1294E-19				FeO	
+ 2.9713E-33				O3)	
+ 0.37792				mol FeS_solid	
(33.224 gram, 0.37792 mol)					

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.

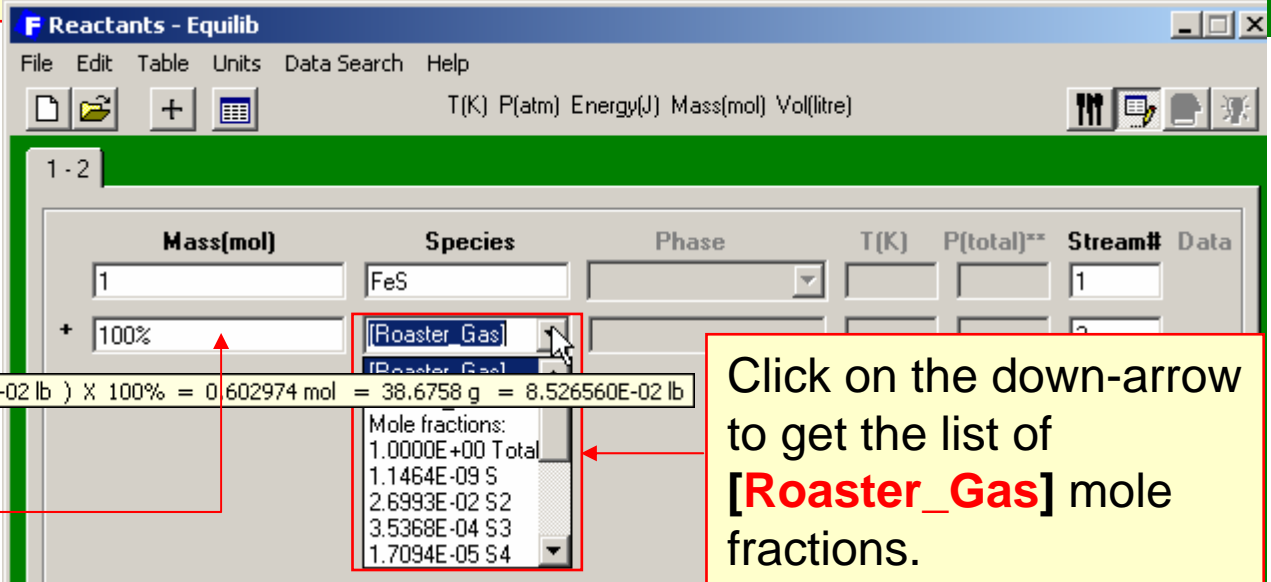
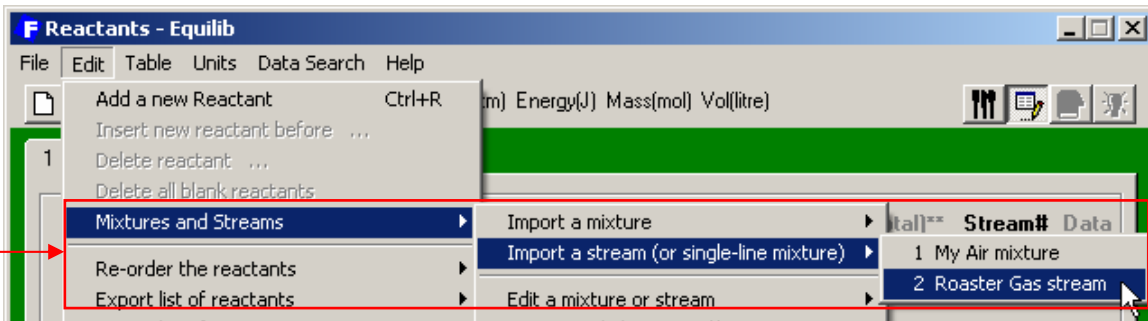
All of these **actions** take place in the **Reactants screen** of the *Equilib* module.

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: **Edit > Mixtures and Streams > Import a single-line mixture or stream > 2 Roaster Gas stream**



Click on the down-arrow to get the list of **[Roaster_Gas]** mole fractions.

Point cursor to display details on the Mass.

Changing the **Mass input** of the stream

Changing input to 0.5 mole.

The screenshot shows the 'Reactants - Equilib' window. The table below is a representation of the data shown in the interface:

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 shows the following composition:

(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 stream automatically changes its composition.

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

The screenshot shows the 'Mixture' program interface. The 'File' menu is open, and the 'Open...' option is highlighted. A yellow callout box points to this menu item with the text: "You can edit a mixture or a stream via the Mixture window: File > Open...>Double-click on **Roaster Gas** stream."

The 'Directory Mixture and Streams' window shows a list of files:

File	Date	Description
1	7Apr09	My Air mixture /
2	20May09	Roaster Gas stre

The 'Mixture and Streams' window displays a 'Reaction Table - 12 rows, 1 reactants' table:

Row	Mass(mol)	Species
1	6.912590183734496E-10	S
2	1.627586755342039E-02	S2
3	2.132597882716795E-04	S3
4	1.030735642836720E-05	S4
5	3.984387295213335E-07	S5
6	1.396627600273019E-07	S6
7	1.265899741689640E-08	S7
8	5.742934254071692E-10	S8
9	1.593614169422414E-05	S0
10	5.840922083737592E-01	S02
11	7.415551479815724E-08	S03
12	2.365736634413287E-03	SS0

At the bottom of the 'Reaction Table' window, there is a text input field for 'total moles' containing the value '0.6029739'. A yellow callout box points to this field with the text: "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

F Mixtures and Streams

File Edit Table Units Data Search Help Mixture or Stream?

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

Reaction Table - 12 rows, 1 reactants

Row	Mass(mol)	Species
1	5.7320808E-10	S
2	1.3496328E-02	S2
3	1.7683998E-04	S3
4	8.5471000E-06	S4
5	3.3039467E-07	S5
6	1.1581161E-07	S6
7	1.0497135E-08	S7
8	4.7621748E-10	S8
9	1.3214620E-05	S0
10	0.4843429	S02
11	6.1491480E-08	S03
12	1.9617239E-03	S0

12 species total moles

FactSage Compound: 1/28 databases c:\FactSage\Mixt2.DAT