LIBPF™

User Manual

Summary

This document is the user's manual for LIBPF™ models version 1.0; it addresses users who want to interact via graphical interfaces with models developed by others (model user).

Prerequisites:

- Basic knowledge of the operating system and a spreadsheet (Microsoft Excel, OpenOffice / LibreOffice Calc);
- Installed, activated and running LIBPF™ application.

For more information see:

- LIBPF_USR_installation for the install and removal procedures;
- LIBPF_USR_activation for the rationale and the functioning of the activation system.

Introduction

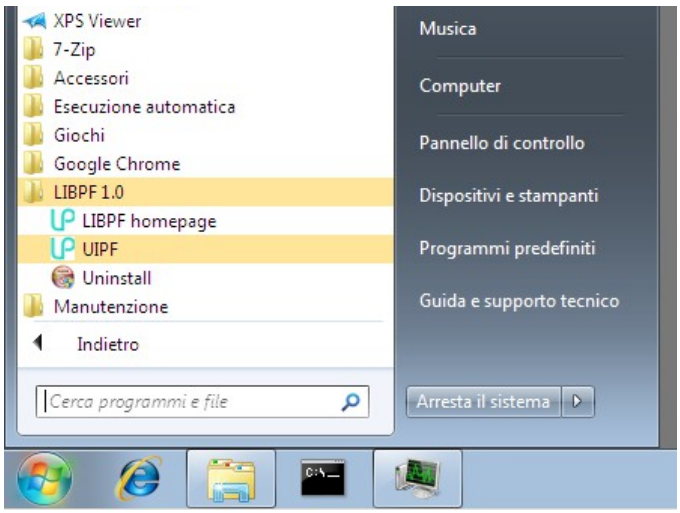
The LIBPF™ (C++ LIBrary for Process Flowsheeting) technology allows you to create an executable and interactive form of the model of a process in various configurations, which then can be deployed as a stand-alone application.
The interaction with the model takes place in a controlled fashion through the LIBPF™ user interface (UIPF: User Interface for Process Flowsheeting). The interface doesn't allow the user to modify the configuration of the process: the present streams and units, their connections and their configurations are fixed once and for all by the developer of the model. An exception can be some specially crafted models that allow the user to tun on and off certain plant units. The interface allows instead to:

- Set the operating parameters and conditions and change the options made available by the developer of the model.
- Perform simulations and sensitivity analyses;
- Save, restore and cancel the cases studied in various conditions;
- Interactively examine the results for streams and units;
- Export the results for all the streams to spreadsheets with Microsoft Excel or OpenDocument ODF formats;
- Export all inputs and results in text or XHTML format.

The LIBPF™ user interface is compatible with several operating systems: Microsoft Windows (Windows Vista / 7 / 8.1 / 10 Technical Preview), Apple OSX (version 10.8 or later) and Linux (e.g. Debian 7, Ubuntu 13 or later); most of the images shown in this manual have been taken on Microsoft Windows Windows 7, but the appearance of the application and its operation does not change on other operating systems.
The LIBPF™ user interface is an internationalized application that supports 12 languages: العربيـة (Modern Arabic, Simplified Chinese, English, French, German, Hebrew, Italian, Japanese, Korean, Portuguese, Russian and Spanish); and the text flows from right to left (for Arabic and Hebrew) as well as from left to right for all other languages.

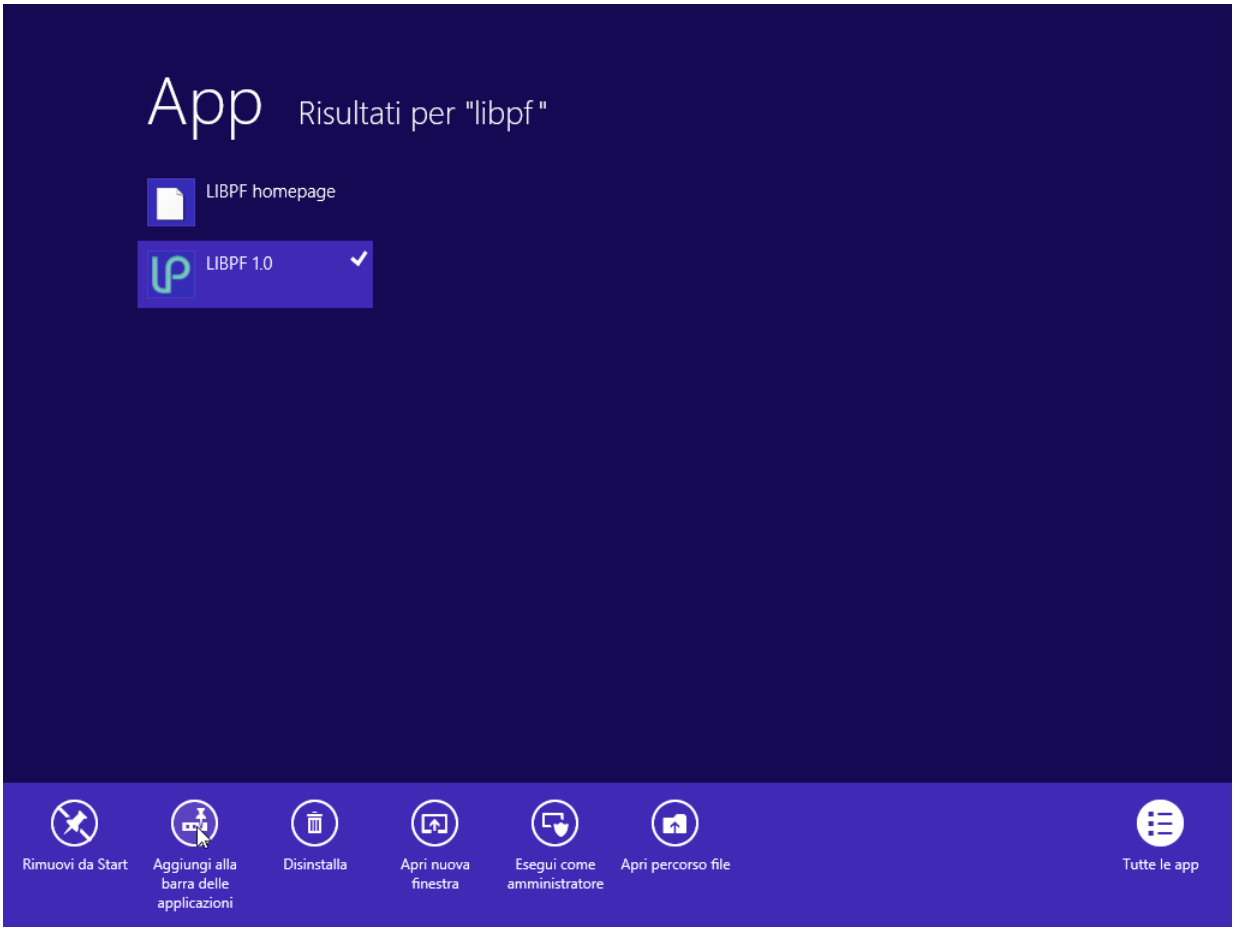
Starting the LIBPF™ user interface

On Linux systems the user interface of LIBPF™ is available as an executable file “UIPF” in the LIBPF_1.0 folder inside the Home user folder (~/LIBPF_1.0). It is possible to move the UIPF file in any favorite position (desktop, other folder, ...) and run it: all data, results and settings are always stored in the kernel directory (~/LIBPF_1.0).
On Microsoft Windows Vista and 7 systems, after installation, the user interface of LIBPF™ is installed in Programs → LIBPF™ 1.0. To launch the user interface, click on UIPF:

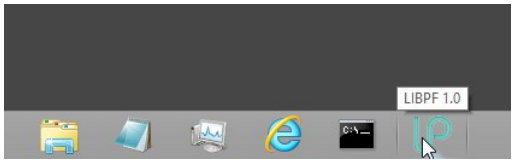


On Windows 8 / 8.1 / 10, the user interface of LIBPF™ runs as a traditional Desktop application, not as a Windows Store App. To start it, go to the Start screen and type "libpf"; it should find the LIBPF™ user interface:

For your convenience, at this point it is better to perform a right mouse button click on the application and select "Add to the application bar" in the lower menu:

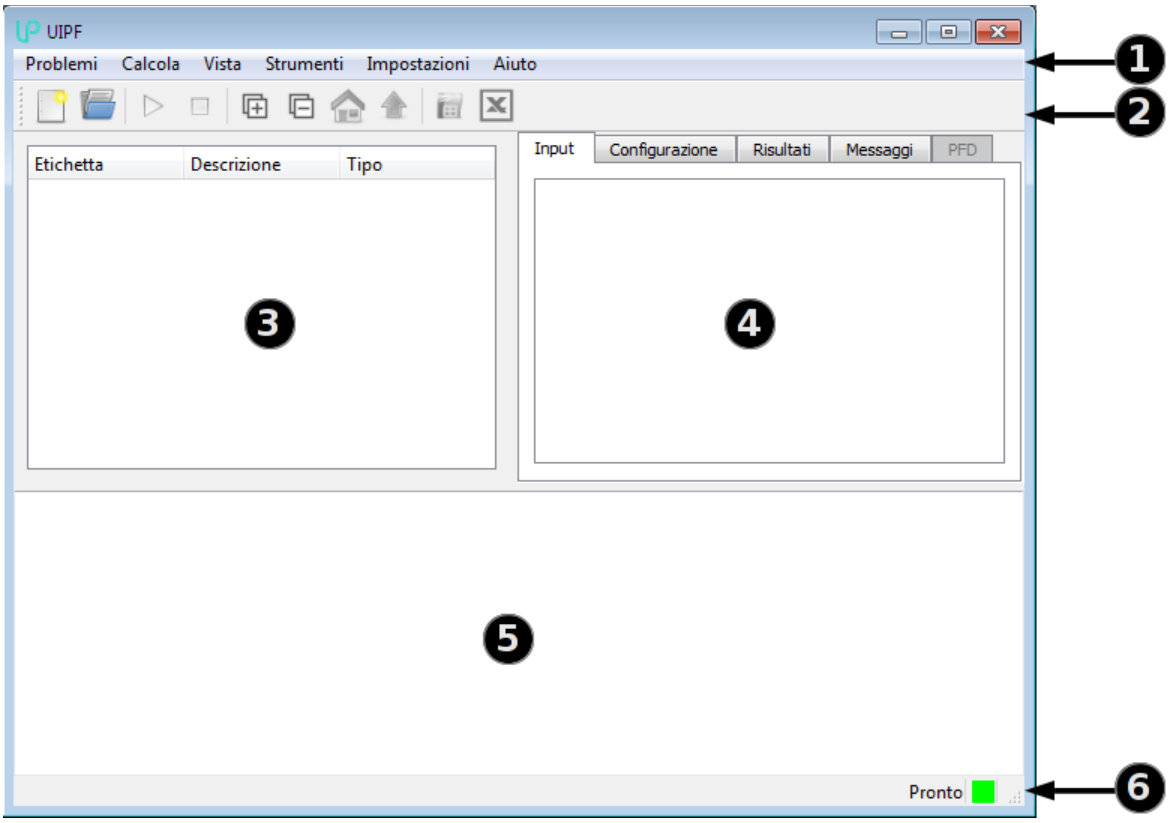


In this way whenever you want to start the LIBPF™ user interface you will find the shortcut in the Desktop application toolbar:



At launch, the interface looks like in the figure below, where you can identify the 6 main areas:

1) Menu bar;
2) Tool bar, which presents a selection of the most frequently used commands;
3) Tree view panel, which shows a structured view of various elements (streams, units, reactions) that make up the process;
4) Details view panel, where you can examine the input and results, and display the connectivity for the flowsheets.
5) Message panel, where diagnostic messages from the calculation engine are shown;
6) Status bar, where confirmation messages appear and where a small box (green in the figure) is shown at the right side, and which becomes red in case of errors.



Case management

Unlike most tools for process simulation, the LIBPF™ user interface does not use files to save the results of the simulations, but relies on a database.
This is possible because the interface does not allow the user to change the configuration of the process, but only the operating parameters and options that have been made available by the developer of the model. The distinction between configuration (fixed for all the simulations of a process) and operating conditions (which differ from one case to another) is analogous to the distinction between classes and the instance of an object in object-oriented programming and is a hallmark of the LIBPF™ technology.

The difference between the conventional approach and the object-oriented one of LIBPF™ is illustrated in the following two tables:

Conventional Approach

General purpose program	Configuration	Operating conditions
Microsoft Excel	Model of process A in conditions 1 [fileA1.xls]	
	Model of process A in conditions 2 [fileA2.xls]	
	Model of process B in conditions 3 [fileA3.xls]	
	Model of process B in conditions 4 [fileA4.xls]	

Object Oriented Approach of LIBPF™

Special purpose program	Configuration	Operating conditions
LIBPF™ application for process A		Conditions 1: case A1
		Conditions 2: case A2
LIBPF™ application for process B		Conditions 3: case B3
		Conditions 4: case B4

The advantages of the object-oriented approach are:

1. Reduces the duplication of information;
2. Reduces the possibility of making errors (e.g. a comparison of process A in conditions 1 and 2 requires that the Microsoft Excel files fileA1.xls and fileA2.xls

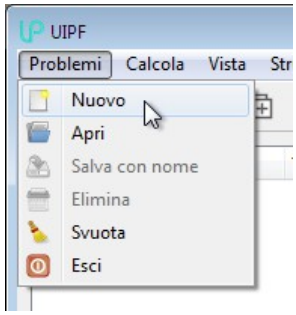
differ only on the operating conditions, and not on the calculation details of the model – but it is easy to make mistakes!);

3. Allows you to systematically update a series of scenarios (a set of cases) with a new version of the process (e.g. with more accurate models).

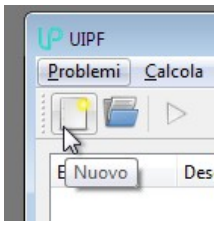
In a typical installation on Microsoft Windows the used database has Access format (although it is not required that Microsoft Access be installed) and is located in the `persistency.mdb` file in the working folder within the current user profile, typically in:
`C:\Program Data\LIBPF 1.0`

Creating a new case

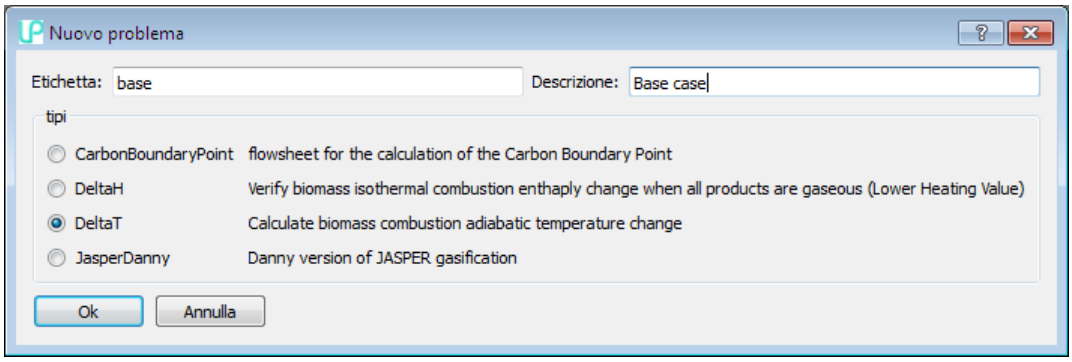
You can create a new case in the LIBPF™ user interface with the *Case* → *New* command from the menu bar:



or with the corresponding button in the toolbar:



The program shows a dialog box which allows you to choose the process configuration (typically a single LIBPF™ application can manage various configurations), and give a name and description to the case:



There are limitations regarding the allowed characters in the label and description fields:

- The first character of the description must be alphabetic, while the subsequent characters may be alphanumeric, space or any of the following characters: `,:-_{}<>[]`.
- The first character of the label must be alphabetic, while the subsequent characters may be alphanumeric, space or any of the following characters: `,-_{}<>` thus compared to the description, the `:[]` characters are specifically excluded.
- By alphabetic character the characters in the a – z, A – Z range are intended (case sensitive), along with all the accented characters (àáâãäåèé ...) and generally all the characters considered alphabetic in the main languages (es. α – ω, A - Ω, A -Я, a – я …);
- By alphanumeric character an alphabetic character or a digit (0 – 9) is intended.

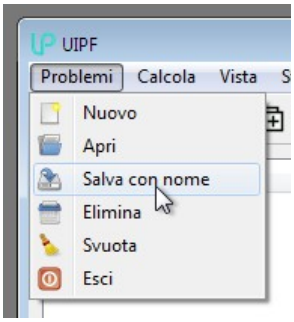
When the user gives the confirmation, the interface starts the computing kernel which instantiates an object of the chosen type (DeltaT in this case) with the name (“base” in this case) and the description (“Base case” in this case) provided by the user, saves it in the database and then opens it. Note that results are not available as no calculation has been performed yet.

At the end of these operations the LIBPF™ user interface is ready for changing the inputs and launching the calculation, see the related chapters Editing input data and Calculation).

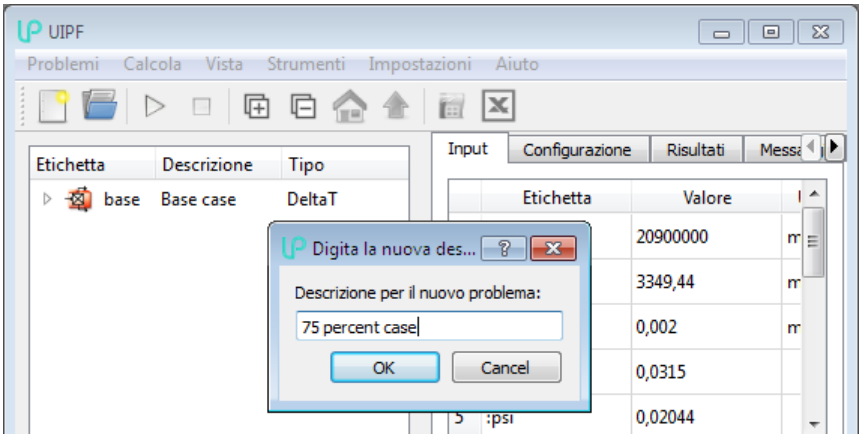
Saving a case with a new name / description

After examining the results, you can decide to create a new case by starting with the current one, with respect to which you may wish to change some operating conditions.

For example if the current case is the “Base case” case, you might want to create a new “75 percent case” case to calculate the operating conditions at reduced load. To do this, use the *Cases* → *Save as* command:



which duplicates the current case in the database, applying the provided description:



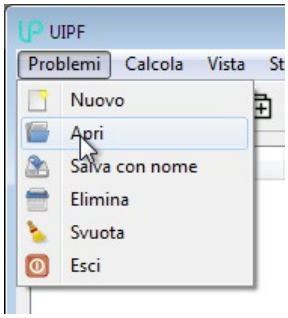
For the characters accepted in the description field, the limitations specified at the Creating a new case chapter apply; a description like “75% case” is not accepted because the % character is not allowed.

Beware: the new case is not immediately loaded in the interface: you must explicitly retrieve the new case, in the manner described in the next chapter Retrieving an existing case.

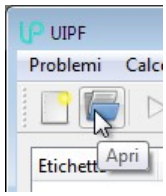
As more fully explained in the Editing input data chapter, any modification of the operating conditions via the graphical interface is immediately applied to the current case. This is why it is important to use the *Save as* command and then immediately load the new case before you start editing anything, otherwise you'll be modifying the current case!

Retrieving an existing case

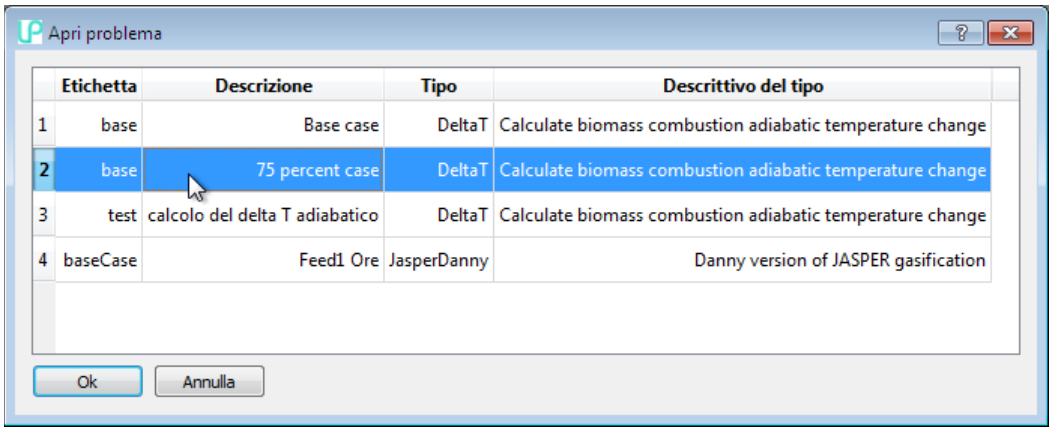
As you proceed with the work, all the generated cases are saved in the database. At any time you can re-open a previously created case with the Cases → Open command:



or with the corresponding button on the toolbar:



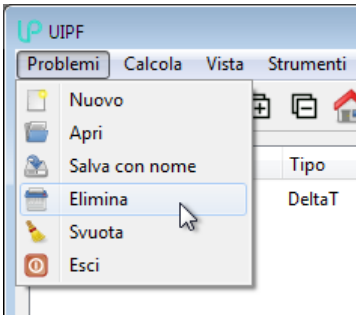
The program will then display a list of the existing cases, from which you can choose the one of interest:



Beware: after loading the case the calculation isn't launched: the cases are saved in the database immediately after being calculated, thus the graphical interface can restore the complete state (input and results).

Troubleshooting

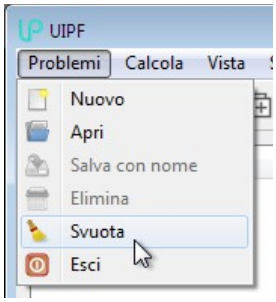
If for any reason the current case is no longer of interest, you can delete it from the database with the *Cases* → *Delete* command:



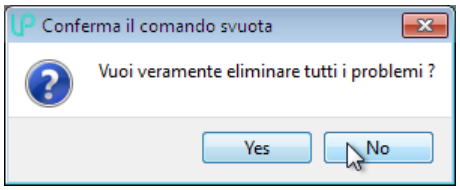
Note: the command is available only after having loaded the case.

Nota bene: the deletion of a case is an irreversible process, and does not require confirmation: proceed with caution!

Also, if there are too many cases in the database, or you want to reset the work done, you can clear the database completely. For this purpose you can use the *Cases* → *Empty* command:



Nota bene: emptying the database completely is an irreversible process and with extensive consequences (e.g. it also deletes cases generated with another LIBPF™ application that are saved in the database, even if they are invisible from the interface), this is why an explicit confirmation is required:



If in doubt, it is advised to make a backup copy of the database (`persistency.mdb` in the working folder location mentioned at page 6 above) manually (copy-past the file) in a separate location (i.e. `Documents\backupDataBases`).

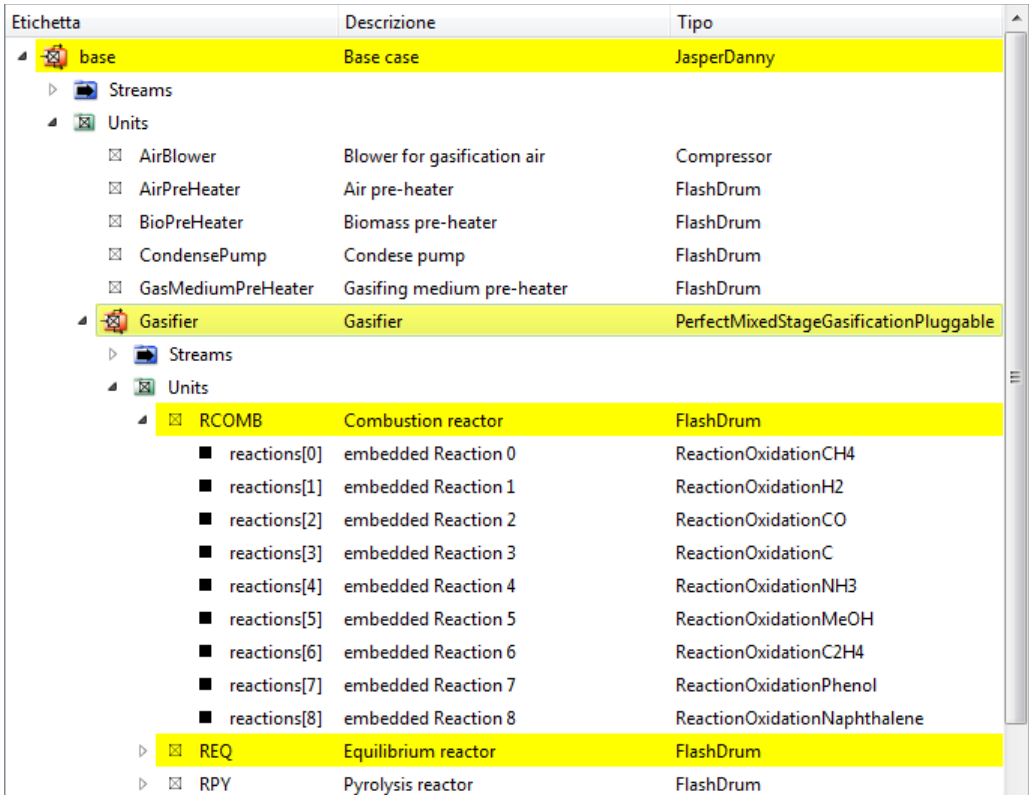
Organization of objects and sub-objects

When a case is opened with the interface, a structured view of various elements (streams, units, reactions) that make up the process is displayed in the tree view panel.
The program uses various icons to indicate the type of object:

Icon	Description
	flowsheets and sub-flowsheets
	the folder containing all the streams
	the folder containing all the units
	a material stream
	a phase (normally contained in a stream)
	a unit (e.g. a compressor or a reactor)
	a chemical reaction
	a multi-reaction (a particular type of reaction that shifts the species from one stream to another, used in the membrane and fuel cell unit)
?	unknown object (this icon should never appear)

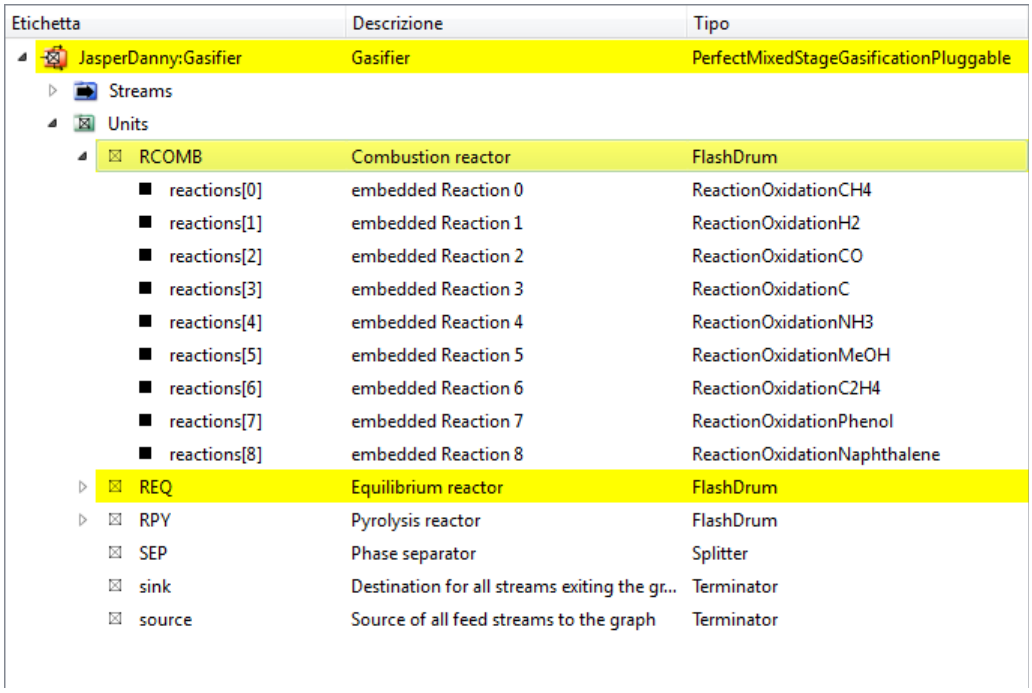
Just after opening a case, the root element (the one at the top) represents the current case. You can navigate through the objects and sub-objects by double-clicking (single clicking on linux systems)on the line in the tree view, which changes the selected object: as you enter the tree structure, it only shows more objects contained in the current object.

For example starting with this kind of view:



Etichetta	Descrizione	Tipo
base	Base case	JasperDanny
Streams		
Units		
AirBlower	Blower for gasification air	Compressor
AirPreHeater	Air pre-heater	FlashDrum
BioPreHeater	Biomass pre-heater	FlashDrum
CondensePump	Condese pump	FlashDrum
GasMediumPreHeater	Gasifing medium pre-heater	FlashDrum
Gasifier	Gasifier	PerfectMixedStageGasificationPluggable
Streams		
Units		
RCOMB	Combustion reactor	FlashDrum
reactions[0]	embedded Reaction 0	ReactionOxidationCH4
reactions[1]	embedded Reaction 1	ReactionOxidationH2
reactions[2]	embedded Reaction 2	ReactionOxidationCO
reactions[3]	embedded Reaction 3	ReactionOxidationC
reactions[4]	embedded Reaction 4	ReactionOxidationNH3
reactions[5]	embedded Reaction 5	ReactionOxidationMeOH
reactions[6]	embedded Reaction 6	ReactionOxidationC2H4
reactions[7]	embedded Reaction 7	ReactionOxidationPhenol
reactions[8]	embedded Reaction 8	ReactionOxidationNaphthalene
REQ	Equilibrium reactor	FlashDrum
RPY	Pyrolysis reactor	FlashDrum

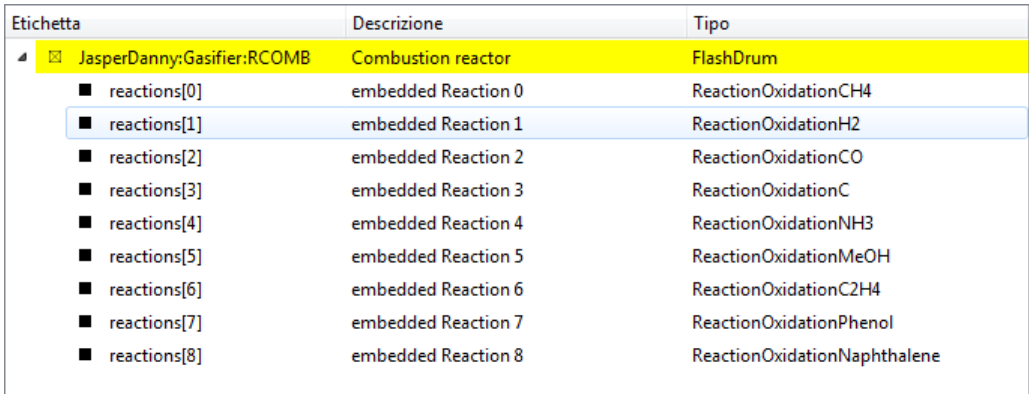
by double-clicking on the Gasifier the view will change this way:



Etichetta	Descrizione	Tipo
JasperDanny:Gasifier	Gasifier	PerfectMixedStageGasificationPluggable
Streams		
Units		
RCOMB	Combustion reactor	FlashDrum
reactions[0]	embedded Reaction 0	ReactionOxidationCH4
reactions[1]	embedded Reaction 1	ReactionOxidationH2
reactions[2]	embedded Reaction 2	ReactionOxidationCO
reactions[3]	embedded Reaction 3	ReactionOxidationC
reactions[4]	embedded Reaction 4	ReactionOxidationNH3
reactions[5]	embedded Reaction 5	ReactionOxidationMeOH
reactions[6]	embedded Reaction 6	ReactionOxidationC2H4
reactions[7]	embedded Reaction 7	ReactionOxidationPhenol
reactions[8]	embedded Reaction 8	ReactionOxidationNaphthalene
REQ	Equilibrium reactor	FlashDrum
RPY	Pyrolysis reactor	FlashDrum
SEP	Phase separator	Splitter
sink	Destination for all streams exiting the gr...	Terminator
source	Source of all feed streams to the graph	Terminator

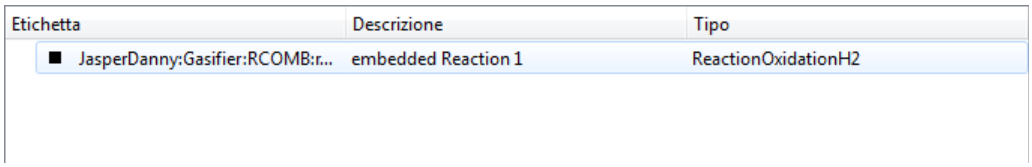
note the full path to the object: `JasperDanny:Gasifier;` in the full paths towards the variables the colon character is used (:) to separate objects from the sub-objects, and period (.) to separate the object from the variable.

Continuing the examination of the sub-objects contained by the Gasifier, by double-clicking on RCOMB the tree view will become:



Etichetta	Descrizione	Tipo
JasperDanny:Gasifier:RCOMB	Combustion reactor	FlashDrum
reactions[0]	embedded Reaction 0	ReactionOxidationCH4
reactions[1]	embedded Reaction 1	ReactionOxidationH2
reactions[2]	embedded Reaction 2	ReactionOxidationCO
reactions[3]	embedded Reaction 3	ReactionOxidationC
reactions[4]	embedded Reaction 4	ReactionOxidationNH3
reactions[5]	embedded Reaction 5	ReactionOxidationMeOH
reactions[6]	embedded Reaction 6	ReactionOxidationC2H4
reactions[7]	embedded Reaction 7	ReactionOxidationPhenol
reactions[8]	embedded Reaction 8	ReactionOxidationNaphthalene

and lastly by double clicking on reactions[1] only the current object will be shown (as the reaction does not contain sub-objects):

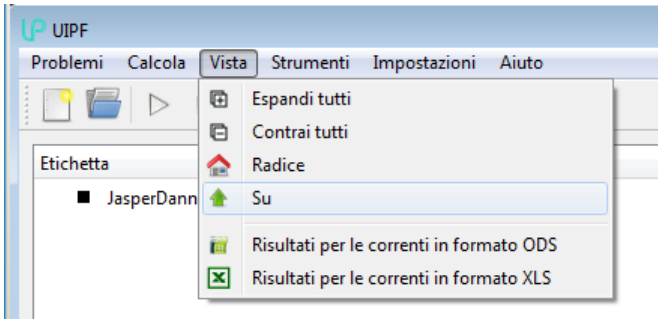


Etichetta	Descrizione	Tipo
JasperDanny:Gasifier:RCOMB:r...	embedded Reaction 1	ReactionOxidationH2

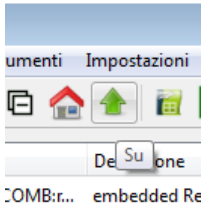
note the full path to the object: `JasperDanny:Gasifier:RCOMB:reactions[1]`; for the vectorial objects or variables the square brackets [] suffix operator selects the object of interest with an integer index starting from zero, for example reactions[0] is the first reaction and x[5] is the sixth mole fraction.

The Stream folder contains Stream-type objects each with the thermodynamical state (T, P) and the Phases as sub-objects, both the separate phases that compose the material and the total phase (if there is more than one phase). The Units folder contains sub-flowsheets and unit operations, each with its operating specifications and key performance data (deltaP, duty, deltaH, deltaS, efficiencies, …). Unit operations can also contain the reactions with their stoichiometric coefficients, equilibrium constants and rate of conversion.

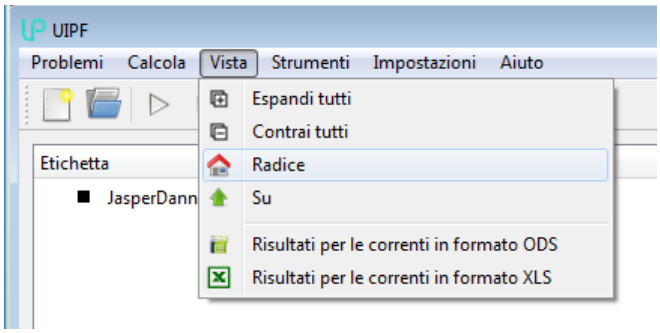
To go in the structure up with a single level, you can use the *View* → *Up* command from the menu bar:



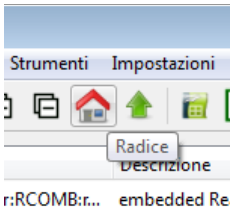
or the corresponding button in the toolbar:



To go up again to the highest level in the structure you can use the *View → Root* command in the menu bar:



or the corresponding button in the toolbar:



Once the object of interest selected, you can examine the details in the panel at the right (details view) which has five tabs:

- Input: user-specified parameters, read-write
- Configurations: enable and disable select additional equations, read-write
- Results: selection of key results, read-only

- Messages: warnings and errors, read-only
- and PFD (Process Flow Diagram), clickable.

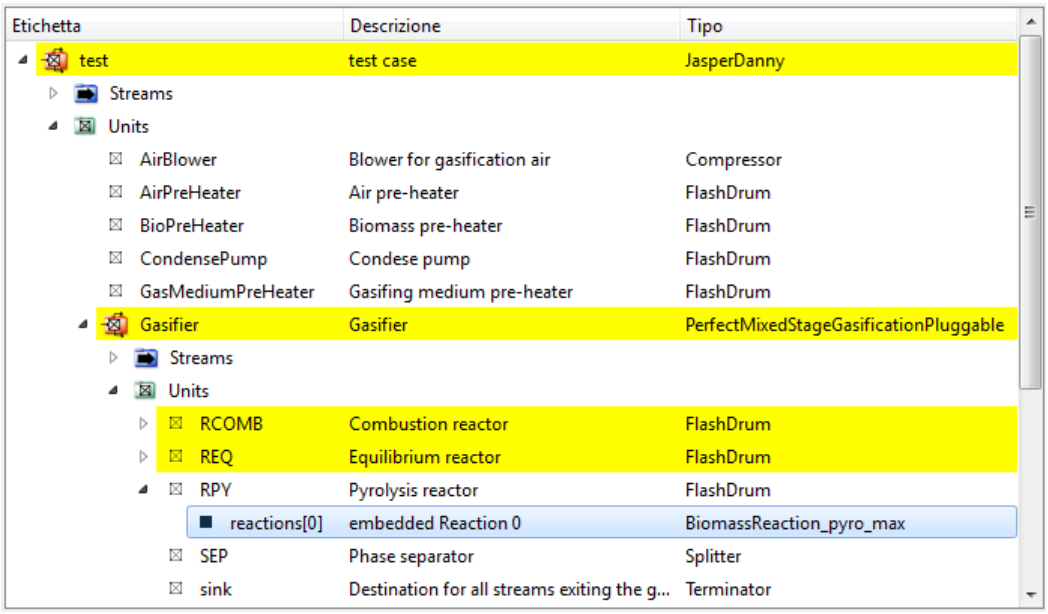
The last tab is active only for flowsheets and sub-flowsheets, and allows to see their process scheme and zoom in or out, and to examine the sub-objects by interactively clicking on the units or streams in the PFD view: the effect is equivalent to a double click on the corresponding object in the tree view on the left.

Simulation

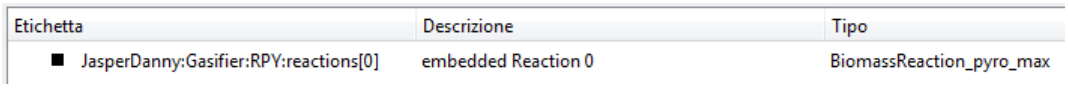
Editing input data

The user interface allows you to set the operating parameters and conditions and change the options that have been made available by the developer of the model. This implies that some input parameters could be inaccessible, because the developer of the model considered them unattractive or even dangerous to handle (e.g. for the stability, accuracy and convergence of the model).

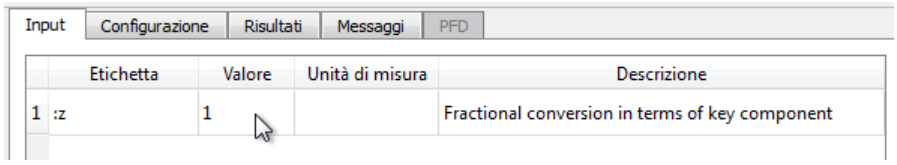
With these limitations, editing is very straightforward: just browse the tree view and identify the stream, unit, sub-flowsheet or reaction you want to edit, and double-click. For example if you want to change an input parameter relative to the reaction[0] reaction of `BiomassReaction_pyro_max` type in the `RPY` unit of `FlashDrum` type found in the `Gasifier` sub-flowsheet of `PerfectMixedStageGasificationPluggable type`, just browse the tree view and double click on the Gasifier:RPY:reactions[0] object:



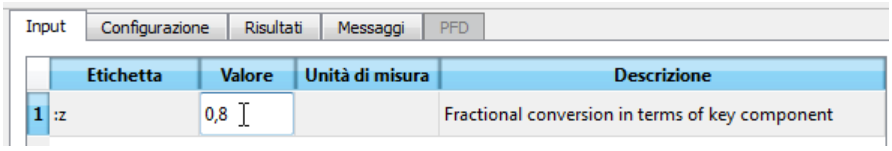
so that you change the tree view, which shows now the current object:



The details view panel now shows a filtered view of the details relative to the selected reaction; particularly clicking on the Input tab the input variables that can be manipulated (only one in this case, the conversion) are shown:



At this point just click in the box and type in the new value:



The change becomes effective after you press Enter or click on another element in the user interface (i.e. removing the focus from the input field).

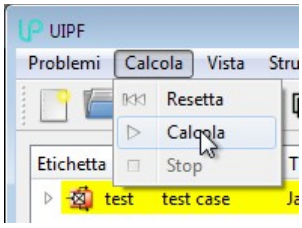
Any change made to the operating conditions carried out this way via the graphical interface is immediately updated in the database with reference to the current case. For this reason explicitly saving the changes as we are used to do in other programs isn't necessary: the *Cases → Save* does not even exist, there is instead *Cases → Save as*, which is used to create a copy of the current case (see the Saving a case with a new name / description related chapter).

Calculation

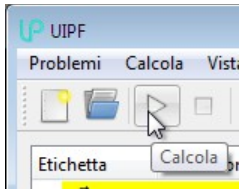
When a new case is created, results are not available as no calculation has been performed yet (see Creating a new case). Also if an existing case is loaded (see Retrieving an existing case) or the current case is edited (see precedent chapter Editing input data), you need to explicitly launch the calculation.

This logic is advantageous if the simulation runs are of considerable duration: if the calculation started automatically after each change, this could render the graphical interface interface unresponsive.

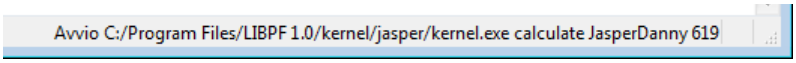
In any case you can launch the calculation of the current case with the *Calculate* → *Calculate* command:



or with the corresponding button in the toolbar:



The calculation is delegated from the graphical interface to an executable, the calculation kernel, which is launched as a separated process, as you can see from the notice indicated in the status bar at the bottom right.



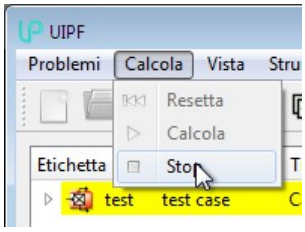
During the calculation in the bottom panel (of the messages) the diagnostic messages coming from the kernel are shown in real time, in order to monitor the progress of the calculation. A typical trace in case of success would be:

```
main * Define components
main * Define flowsheet
main * Retrieving 619 from persistent storage database
main * Define cut streams convergence
main * Starting computation
FlowSheet<class ZeroZero>::calculate * Iter = 0 Error = 0.023535
FlowSheet<class ZeroZero>::calculate * Iter = 1 Error = 0.00105955
FlowSheet<class ZeroZero>::calculate * Iter = 2 Error = 5.08785e-005
FlowSheet<class ZeroZero>::calculate * Iter = 3 Error = 3.75563e-006
FlowSheet<class ZeroZero>::calculate * Iter = 4 Error = 1.22477e-006
FlowSheet<class ZeroZero>::calculate * Iter = 5 Error = 4.54359e-007
main * Computation complete
main * Updating results to persistent storage
main * Save stream table in ODF format
main * Program exits correctly
```

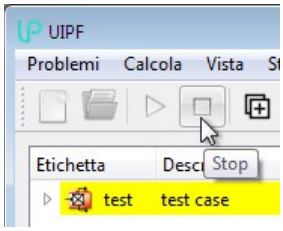
If instead during the calculation errors occur, these are highlighted in red in the messages panel:

```
===== Logging error negative material flow in test:AirToICE
===== Logging error exceeded maximum iterations limit in test:Gasifier:REQ
===== Logging error Flash convergence failure in FlashDrumBase::calculate; in test:Gasifier:REQ
FlowSheet<class ZeroZero>::calculate * Iter = 9 Error = 1.27904e-006
===== Logging error exceeded maximum iterations limit in test:Gasifier:REQ
===== Logging error Flash convergence failure in FlashDrumBase::calculate; in test:Gasifier:REQ
===== Logging error negative material flow in test:AirToICE
===== Logging error exceeded maximum iterations limit in test:Gasifier:REQ
===== Logging error Flash convergence failure in FlashDrumBase::calculate; in test:Gasifier:REQ
FlowSheet<class ZeroZero>::calculate * Iter = 10 Error = 6.39521e-007
main * Computation complete
main * Updating results to persistent storage
===== Logging error exceeded maximum iterations limit in test:Gasifier:REQ
main * Save stream table in ODF format
main * Program exits correctly
```

In these anomalous situations the duration of the calculation could go on for too long, and seen the encountered errors the results will certainly be devoid of interest; if needed in these cases you can stop the calculation using the *Calculate* → *Stop* command:



or with the corresponding button in the toolbar:

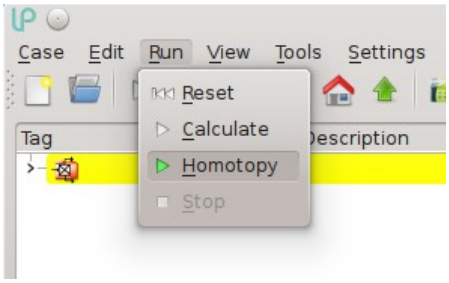


At the end of every calculation you can examine the results in the manner specified in chapter Examining the results.

Homotopy

Homotopy is a globally convergent numerical continuation method for solving systems of non-linear equations. With homotopy, to solve a complex problem, you solve first a simpler problem and then continuously transform it so that its solution is transformed into the solution of the complex problem. During this transformation it is possible to track what happens to the equations and to the solution, so that the speed of the deformation can be adapted.

Within the LIBPF™ User Interface it is possible to to solve in homotopy mode:

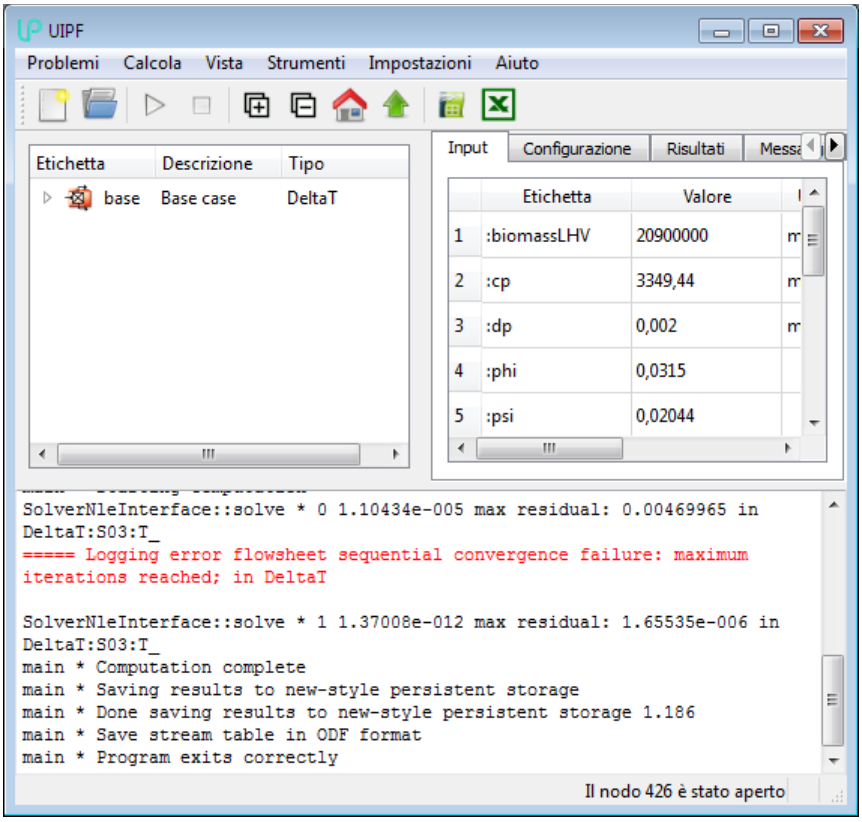


This solution mode is useful when the process is very sensitive to changes to certain input parameters, or when the desired step change for those parameters is relatively large. In Homotopy mode all the input variables whose values have been changed by the user since the last computation are moved simultaneously and gradually from the previous state to the new desired state, repeatedly solving the model for the intermediate values.

Examining the results

Calculation status

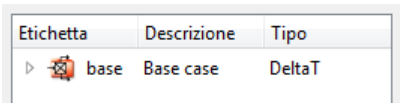
At the end of a calculation or even after having created a new case the user interface will display something similar to this figure:



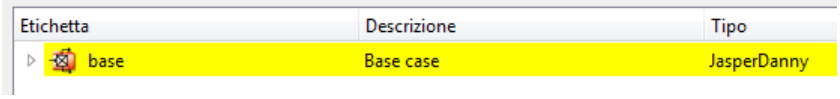
Firstly note in the status bar at the bottom right the “Node 426 has been opened” notification: this number is internally used by the database to uniquely identify the current case.

In the top left panel (tree view) the program uses color codes to indicate at a glance the status of the last calculation:

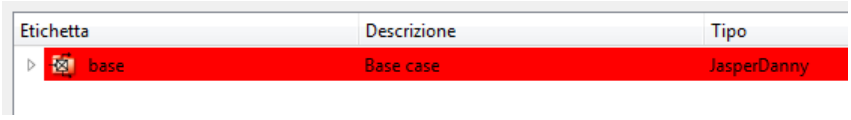
- white indicates: no error nor warnings:



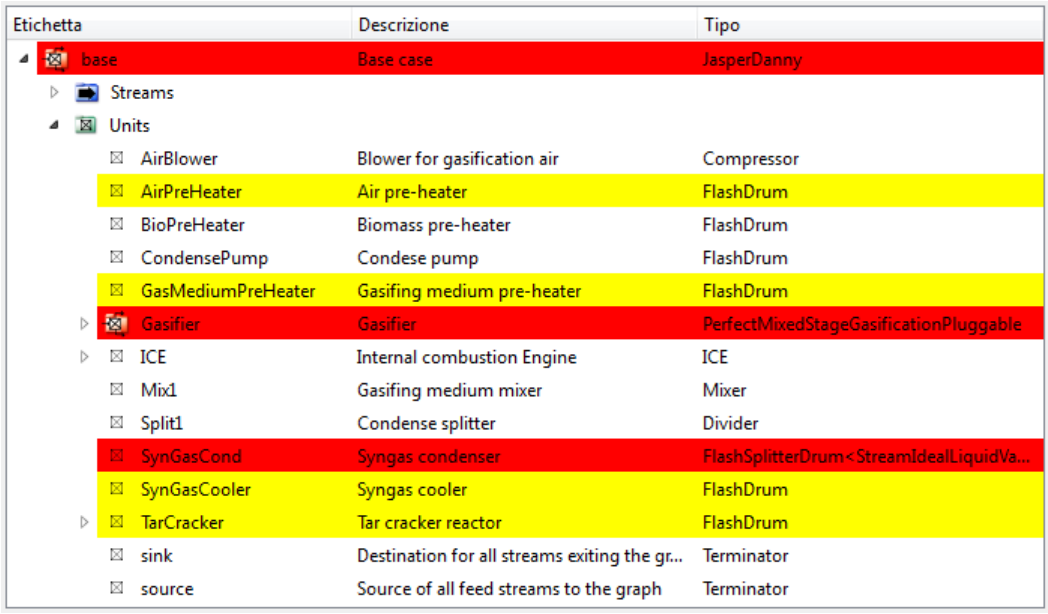
- yellow indicates: there are warnings:



- red indicates: there are errors:



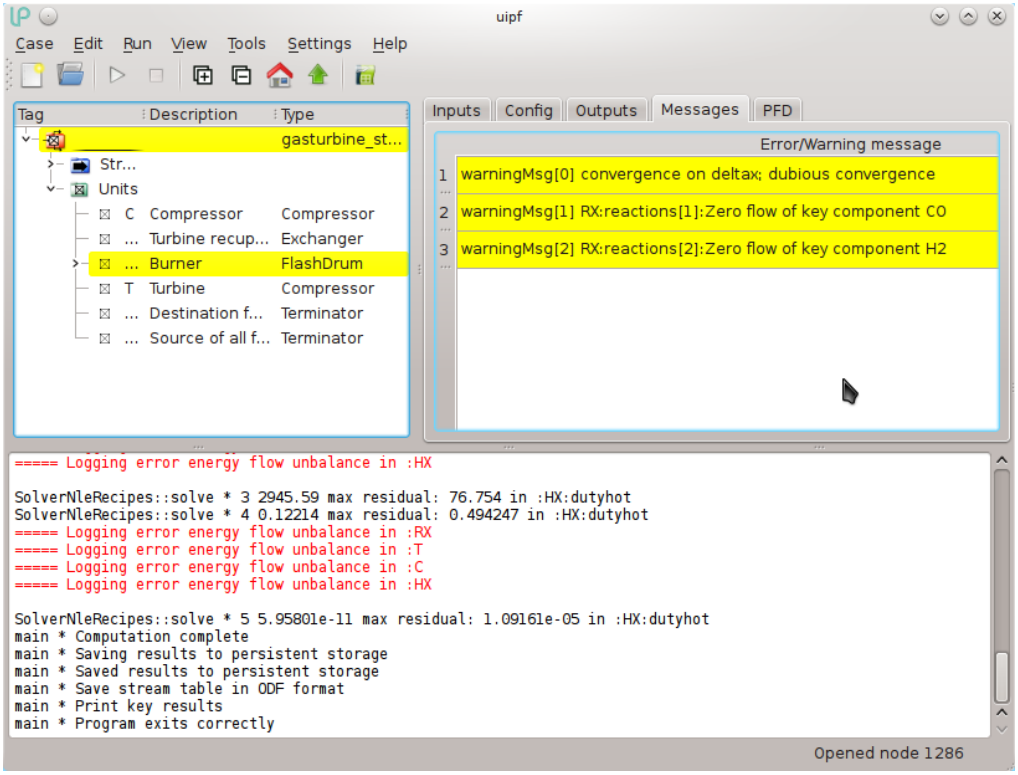
In case of warnings or errors the color codes are displayed on each object to make the search for the cause easier:



Etichetta	Descrizione	Tipo
base	Base case	JasperDanny
Streams		
Units		
AirBlower	Blower for gasification air	Compressor
AirPreHeater	Air pre-heater	FlashDrum
BioPreHeater	Biomass pre-heater	FlashDrum
CondensePump	Condese pump	FlashDrum
GasMediumPreHeater	Gasifing medium pre-heater	FlashDrum
Gasifier	Gasifier	PerfectMixedStageGasificationPluggable
ICE	Internal combustion Engine	ICE
Mix1	Gasifing medium mixer	Mixer
Split1	Condense splitter	Divider
SynGasCond	Syngas condenser	FlashSplitterDrum<StreamIdealLiquidVa...
SynGasCooler	Syngas cooler	FlashDrum
TarCracker	Tar cracker reactor	FlashDrum
sink	Destination for all streams exiting the gr...	Terminator
source	Source of all feed streams to the graph	Terminator

From this example you can see that the (“base”) case contains errors (red line) because the Gasifier and SynGasCond sub-objects contain errors. The AirPreHeater, GasMediumPreHeater, SynGasCooler and Tar Cracker contain warnings (yellow lines), but the errors prevail in determining the global state of the case.

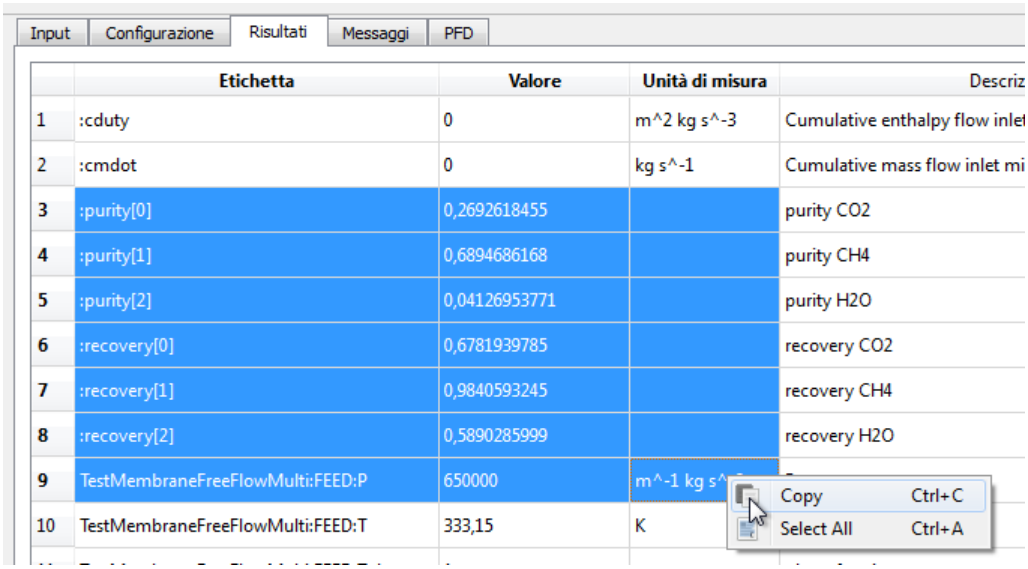
Details and descriptions about the errors and warnings can be found in the Messages tab for each unit, with the same color conventions of yellow for warnings and red for errors:



Results

You can find the results for various units and streams in the “Results” tabs from the panel at the right (details view) by browsing through the objects and sub-objects as shown in the Organization of objects and sub-objects chapter.

These tables allow selecting a subset of cells or the entire table, and copying that to the clipboard:



For the selection in the screen-shot, the text copied to the clipboard will include the column header and the content of the selected cells, with tabs (character →|) as separators of the fields:

```
Tag→|Value→|Units
:purity[0]→|0,269262→|
:purity[1]→|0,689469→|
:purity[2]→|0,0412695→|
:recovery[0]→|0,678194→|
:recovery[1]→|0,984059→|
:recovery[2]→|0,589029→|
TestMembraneFreeFlowMulti:FEED:P→|650.000→|m^-1 kg s^-2
```

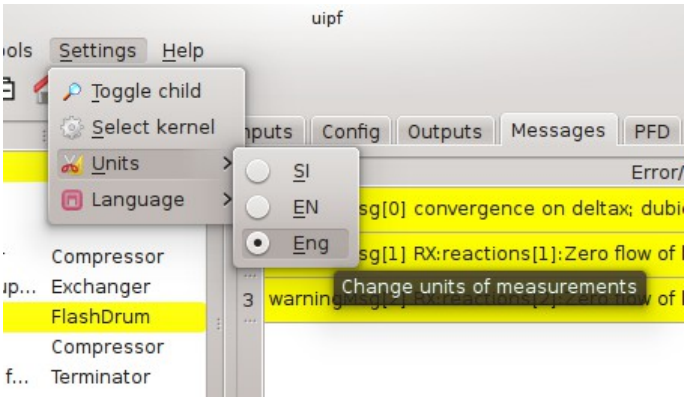
The content of the clipboard can then be directly pasted to a spreadsheet, and the tabs will be interpreted as column separators.

The results for the material streams (material and energy balances) can be exported to a spreadsheeting program such as Microsoft Excel (if available) on the supported Microsoft Windows operating systems, or LibreOffice / OpenOffice (if available) on all supported operating systems, as shown in the following two paragraphs.

Concerning numerical values, the LIBPF™ user interface uses the global system settings for the number formats (comma or dot as decimal separator etc.).

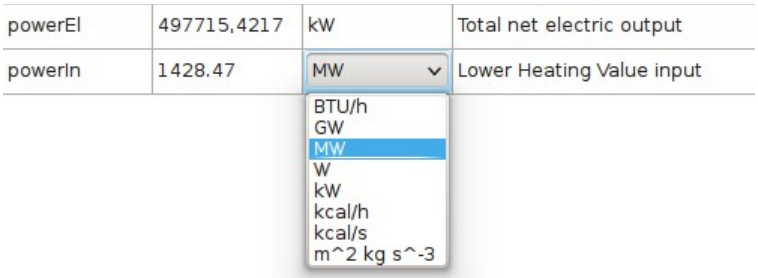
Units of measurement (UOM)

The LIBPF™ user interface currently supports three sets of units of measurements: SI (International System of Units), EN (imperial units) e Eng (engineering units). The default settings is SI, which is also the unit sets internally used by the kernel for all the computations. It is possible to change the units of measurements for all the variables by selecting the menu Settings → Units:



Whenever the global unit setting is changed, all inputs and results are presented in the selected units from that moment on, and the previously set values are converted so that results must actually be unchanged.

Besides these global units of measurements settings, the LIBPF™ user interface also supports setting units for each individual variable, both in input and in output forms. These settings can be changed by pulling down the combo boxes “Units of measurements" found to the right of each variable. As soon as the unit is changed, values are automatically converted.



The supported units of measurements are listed in the following table, grouped by the underlying physical quantity:

acceleration	m/s2
adimensional	
amount	mol
amount flow	kmol/s
	kmol/h
	lbmol/h
	mol/h
	mol/s
	Nm3/h
	Nm3/d
amount specific electric	C/kmol

charge	
amount specific energy	J/kmol
	kJ/kmol
	BTU/lbmol
	kcal/kmol
amount specific entropy	J/(kmol*K)
	J/kmol/K
	kJ/kmol/K
angle	rad
area	m2
	dm2

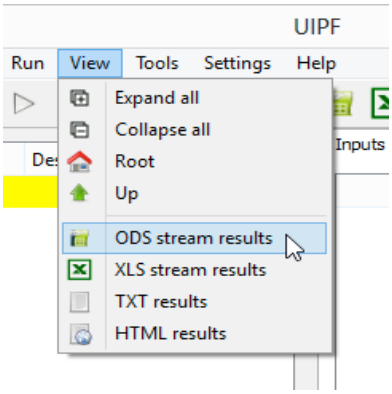
	ft2
	cm2
	mm2
areic current	A/m2
	A/dm2
	A/ft2
	A/cm2
	A/mm2
	mA/cm2
areic electric resistance	ohm*m2
	ohm*cm2
capacitance	F
conductance	S
current	A
density	kg/m3
	mg/m3
	g/m3
	lb/ft3
diffusivity	m2/s
dynamical viscosity	Pa*s
	cP
	mPa*s
electric charge	C
electric potential	V
	mV
electric resistance	ohm
energy	J
	BTU
	mmBTU
	MWh
	kcal
	kWh
energy price	€/J
	€/mmBTU
	$/mmBTU
	$/J
	€/kWh
	€/MWh
	€/kcal
	€/kcal
entropy	J/K
entropy power	W/K
	BTU/h/°F
flow coefficient	kg/m7
force	N
frequency	Hz
heat transfer coefficient	W/(m2*K)
	kcal/(h*m2*K)
	BTU/(h*ft2*F)
	W/m2/K
heat transfer resistance	m2*K/W
inductance	H
inverse of length	1/m
inverse of molecular weight	kmol/kg
inverse of molecular weight	mol/kg
inverse of temperature	1/K
length	m
	ft
	km
	dm
	cm
	mm
	um
length*time	m*s
luminous intensity	cd
magnetic flux	Wb
magnetic flux density	T
mass	kg
	mg
	t
	lb
	g
mass flow	kg/s
	kg/h
	kg/d
	g/d
	t/h
	t/d
	t/yr
	lb/h
mass per unit work	kg/J
mass specific energy	J/kg
	kcal/kg
	BTU/lb
	MJ/kg
	kJ/g
	kJ/kg
	m2/s2
mass specific heat capacity	J/(kg*K)
	kcal/(kg*K)
	BTU/lb/°F
	kcal/kg/K

	J/kg/K
	kJ/kg/K
mass specific volume	m3/kg
molar concentration	kmol/m3
	mol/m3
	lbmol/ft3
	mmol/dm3
	mol/dm3
molar volume	m3/kmol
molecular weight	kg/kmol
	mg/Nm3
	g/Nm3
	lb/lbmol
money	€
permeance	kmol/kg/m
	GPU
power	W
	BTU/h
	kW
	kcal/s
	kcal/h
	GW
	MW
power density	W/m2
pressure	Pa
	MPa
	atm
	bar
	barg
	mbar
	hPa
	kPa
	mmHg
	Torr
	mmH2O
	kg/cm2
	psi
pressure*molar volume squared	Pa*m6/kmol2
resistivity	ohm*m
	ohm*cm
second temperature derivative of density	kg/(m3*K2)
second temperature derivative of pressure	Pa/K2
second temperature derivative of pressure*molar volume squared	Pa*m6/kmol2/K2
second temperature derivative of specific heat	J/(kg*K3)
surface tension	N/m
temperature	K
	°C
	°F
temperature derivative of density	kg/(m3*K)
temperature derivative of pressure	Pa/K
temperature derivative of pressure*molar volume squared	Pa*m6/kmol2/K
temperature derivative of specific heat	J/(kg*K2)
temperature squared/pressure	K2/Pa
temperature/pressure	K/Pa
thermal conductivity	W/(m*K)
	W/m/K
thermal resistivity	m*K/W
thermal resistivity squared	m2*K2/W2
time	s
	min
	h
	d
	yr
VdW a	N*m4*kmol-2
VdW a*n*n	N*m4
velocity	m/s
volume	m3
	ft3
	dm3
	cm3
	mm3
	ul
	ml

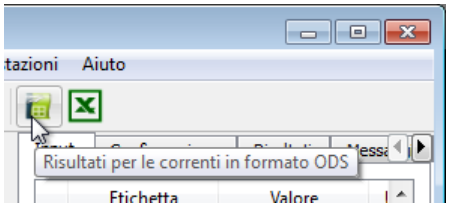
	l	l/h
volume flow	m3/s	
	m3/h	
	ft3/h	

Exporting material and energy balances to LibreOffice / OpenOffice

If a program that can open the OpenDocument ODF format such as LibreOffice or OpenOffice has been installed, you can export all the material and energy balances for the material streams table by using the *View → Results for streams in ODS format* command:

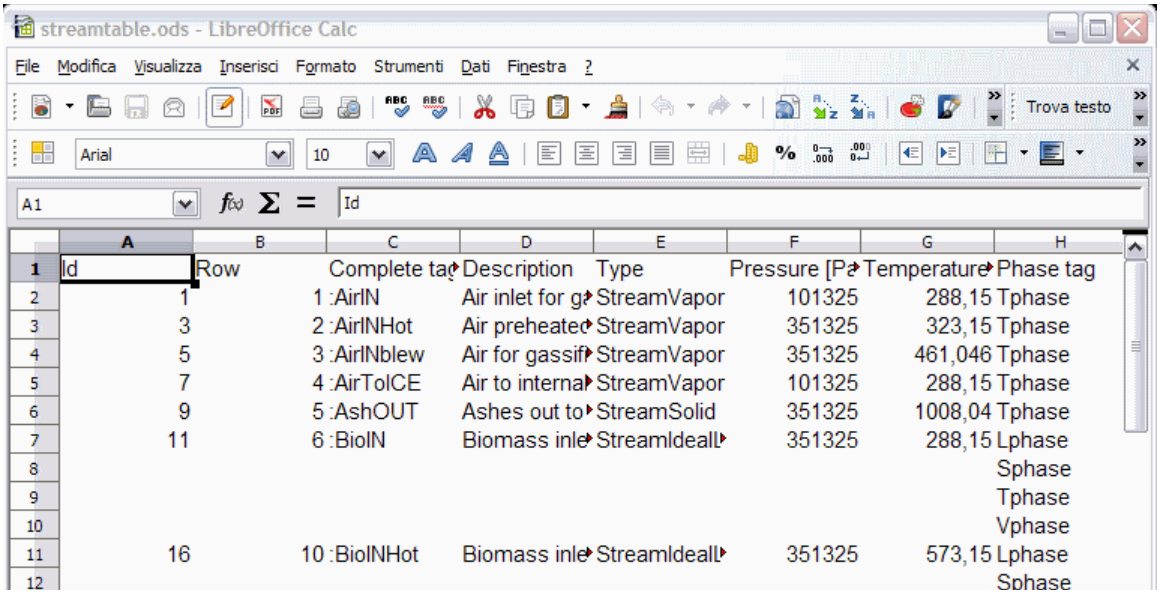


or with the corresponding button in the toolbar:



Note: the command is available only after having carried out the calculation.

Also in this case, the spreadsheet will open in a few seconds:



	A	B	C	D	E	F	G	H
1	Id	Row	Complete tag	Description	Type	Pressure [Pa]	Temperature	Phase tag
2	1		1 :AirIN	Air inlet for g	StreamVapor	101325	288,15	Tphase
3	3		2 :AirINHot	Air preheated	StreamVapor	351325	323,15	Tphase
4	5		3 :AirINblew	Air for gassif	StreamVapor	351325	461,046	Tphase
5	7		4 :AirTolCE	Air to interna	StreamVapor	101325	288,15	Tphase
6	9		5 :AshOUT	Ashes out to	StreamSolid	351325	1008,04	Tphase
7	11		6 :BioIN	Biomass inle	StreamIdeall	351325	288,15	Lphase
8								Sphase
9								Tphase
10								Vphase
11	16		10 :BioINHot	Biomass inle	StreamIdeall	351325	573,15	Lphase
12								Sphase

The operating logic of this command is very different of the one described in the previous chapter, Errore: sorgente del riferimento non trovata; in this case no macro is run in {Libre, Open}Office, but rather the streamtable.ods file is directly generated starting from certain files produced by the calculation kernel (particularly contents.xml, which is produced at the end of each calculation). This implies that the `streamtable.ods` file is rewritten each time, thus you can't keep a “formatted” sheet that presents the same results properly formatted, as in Microsoft Excel. In addition due to the inner workings of LIBPF™, the data for each stream and each phase is arranged by row instead of column as in the case of Microsoft Excel, which makes reading difficult.

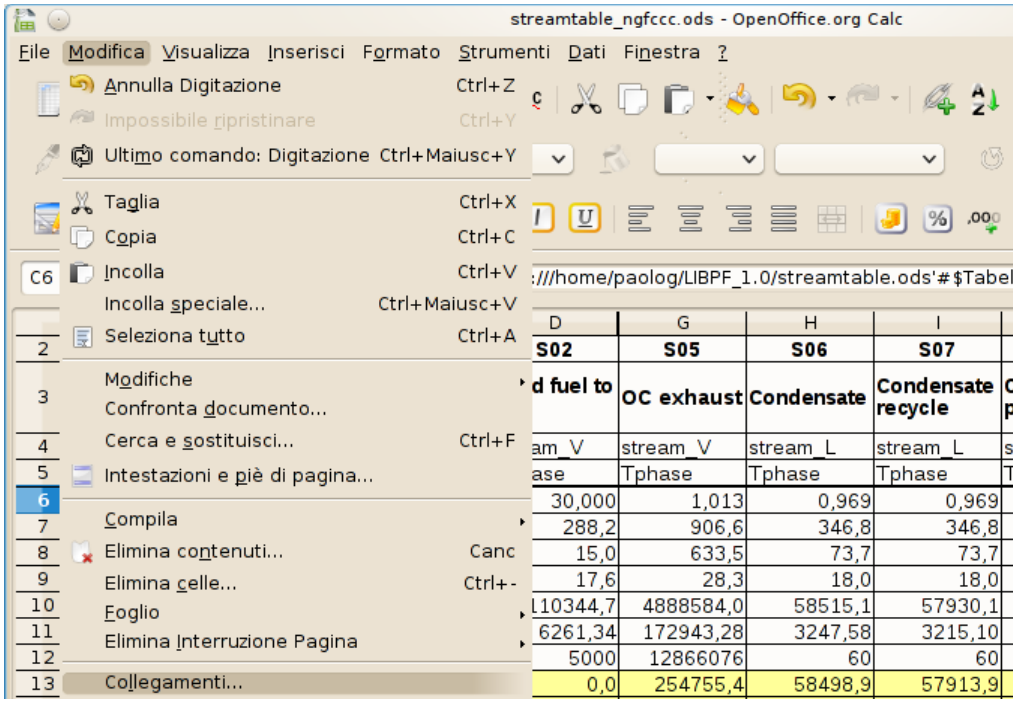
The approach to create a readable format is to create an independent {Libre, Open}Office file e.g. formatted.ods and take the fields of interest by creating a link between the formatted.ods and streamtable.ods files, for example:

```
=file:///home/paolog/LIBPF_1.0/streamtable.ods'#$Tabella1.$A$1
```

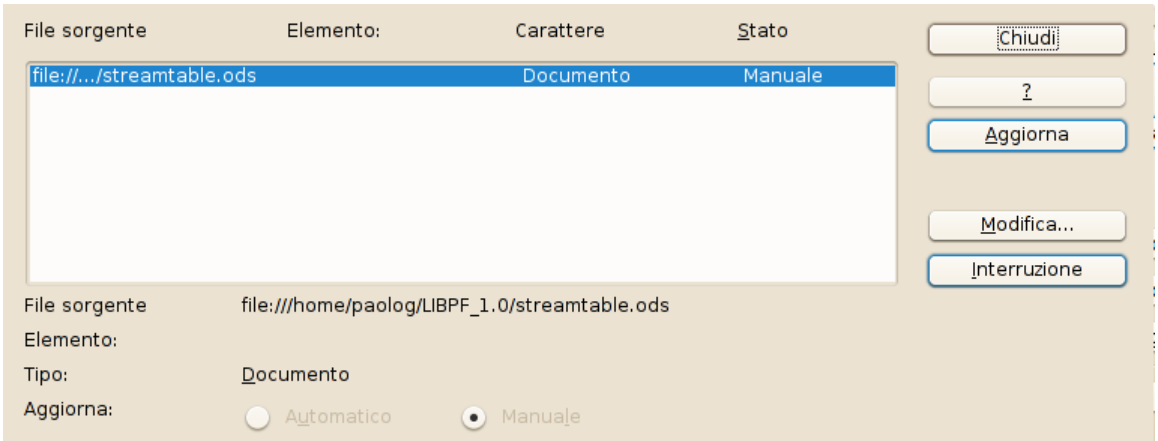
The {Libre,Open}Office `INDEX(reference, row, column)` function may be useful, as it allows you to switch from a row view to a column view.

By creating such connections, the `formatted.ods` file will remain permanently linked with the `streamtable.ods` file; at each new run you will be able to update the `formatted.ods` file in four steps:

1) Using the *View → Results for streams in ODS format* command in the LIBPF™ user interface;
2) Closing the this way rebuilt `streamtable.ods` file which will open automatically (examining or editing this file is not of interest);
3) Using the Edit → *Links* command for `formatted.ods` in {Libre,Open}Office:

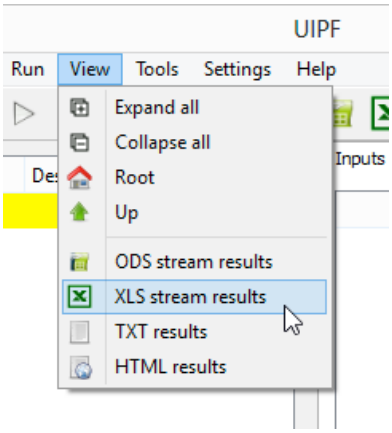


4) Clicking on the “Update” button and closing the dialog box:

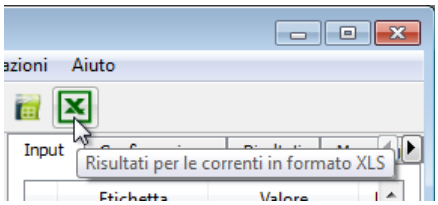


Exporting material and energy balances to Microsoft Excel

On supported Microsoft Windows operating systems, if the Microsoft Excel is installed, you can export all the material and energy balances for the material streams table by means of the *View → Results for streams in XLS format* command:

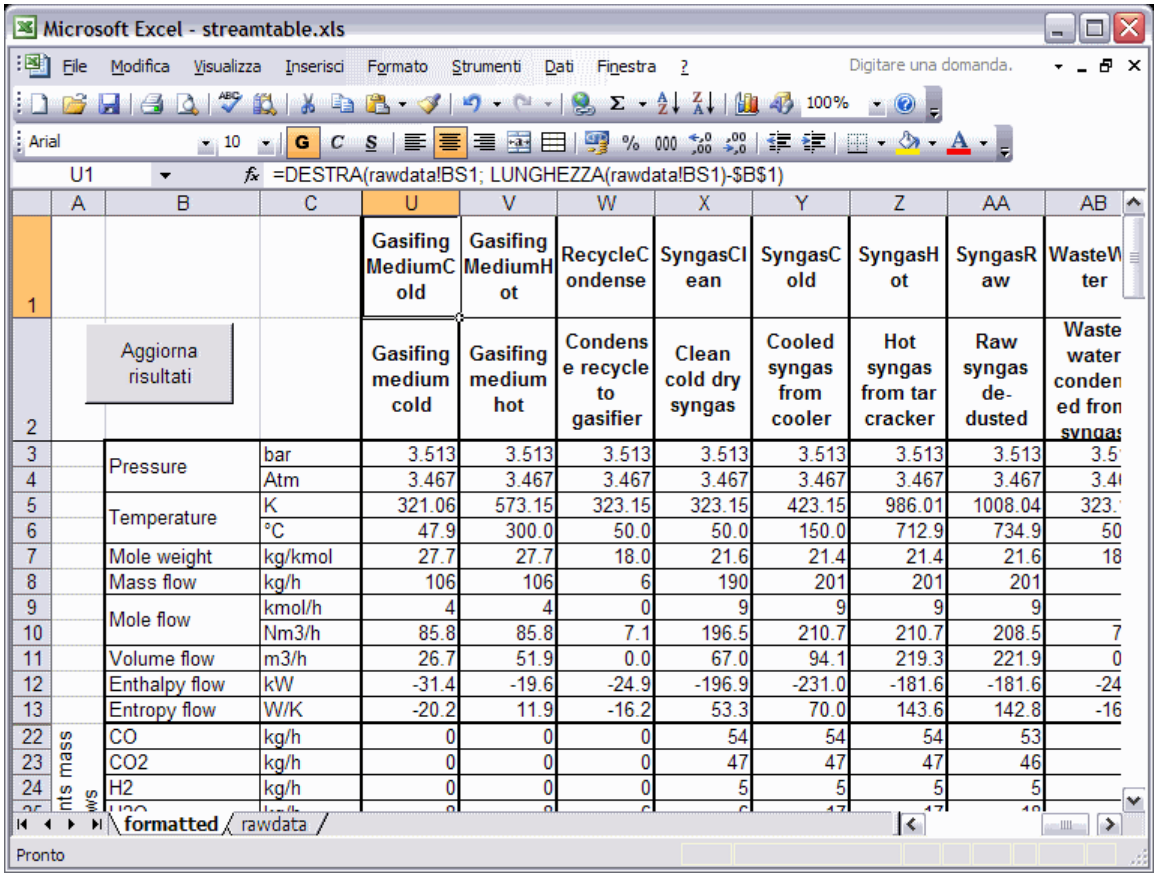


or with the corresponding button in the toolbar:



This command opens the `streamtable.xls` file in Microsoft Excel, and launches a macro written in Visual Basic for Applications which reads the needed values from the Microsoft Access database loading them in the “rawdata” sheet of the file.

The “formatted” sheet presents the same results properly formatted:



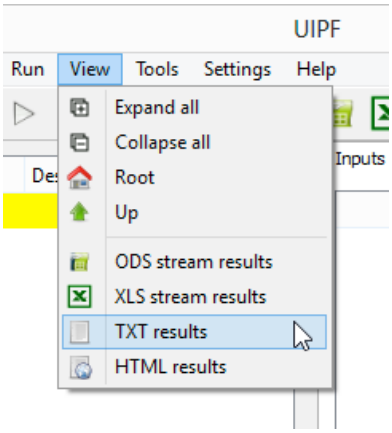
				U	V	W	X	Y	Z	AA	AB
1				Gasifing MediumCold	Gasifing MediumHot	RecycleCondense	SyngasClean	SyngasCold	SyngasHot	SyngasRaw	WasteWater
2				Gasifing medium cold	Gasifing medium hot	Condense recycle to gasifier	Clean cold dry syngas	Cooled syngas from cooler	Hot syngas from tar cracker	Raw syngas de-dusted	Waste water conden ed fron syngas
3		Pressure	bar	3.513	3.513	3.513	3.513	3.513	3.513	3.513	3.5
4			Atm	3.467	3.467	3.467	3.467	3.467	3.467	3.467	3.4
5		Temperature	K	321.06	573.15	323.15	323.15	423.15	986.01	1008.04	323.
6			°C	47.9	300.0	50.0	50.0	150.0	712.9	734.9	50
7		Mole weight	kg/kmol	27.7	27.7	18.0	21.6	21.4	21.4	21.6	18
8		Mass flow	kg/h	106	106	6	190	201	201	201	
9		Mole flow	kmol/h	4	4	0	9	9	9	9	
10			Nm3/h	85.8	85.8	7.1	196.5	210.7	210.7	208.5	7
11		Volume flow	m3/h	26.7	51.9	0.0	67.0	94.1	219.3	221.9	0
12		Enthalpy flow	kW	-31.4	-19.6	-24.9	-196.9	-231.0	-181.6	-181.6	-24
13		Entropy flow	W/K	-20.2	11.9	-16.2	53.3	70.0	143.6	142.8	-16
22	nts mass	CO	kg/h	0	0	0	54	54	54	53	
23		CO2	kg/h	0	0	0	47	47	47	46	
24	ws	H2	kg/h	0	0	0	5	5	5	5	

Beware to the displayed columns in the "formatted" sheet: it may be necessary to extend or reduce the number of those columns appropriately to handle flowsheet with more or less streams. If it is necessary to increase the number of formatted columns, select the last column to the right then click on the fill icon in the top-right corner then pull to the right; after that, remove the columns which display no stream name.

You can leave the Microsoft Excel window open and press the “Update results” button to re-run at any time (e.g. after a new calculation) the macro: this file will keep pointing to the object that was open in the LIBPF™ user interface at the moment when the command of opening Excel has been given.

Exporting all data to a text file

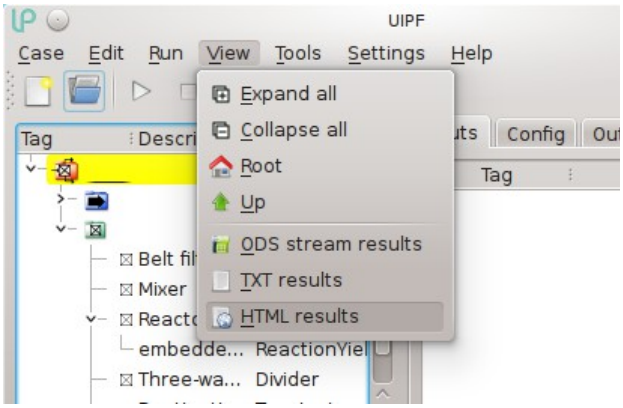
It is possible to export all the data for the currently open object and all its sub-objects, saving them to a text file (.txt). This functionality is available in the “View” menu by clicking on “TXT results”:



When this command is clicked, the current model (more precisely the node currently open in the tree view) is exported to a plain text file named "ID.txt" where ID is the model identifier in the database. The generated text file is automatically opened and displayed in the Operating System default application for opening text files (i.e. Notepad).

Exporting all data as XHTML

It is possible to export all the data for the currently open object and all its sub-objects, saving them in HTML format. This functionality is available in the "View" menu by clicking on "HTML results":



When this command is clicked, the current model (more precisely the node currently open in the tree view) is exported to a number of separate XML files, which are placed in a temporary directory together with a dozen auxiliary files.

The XHTML file named "index.xhtml" is automatically opened by the Operating System default application for opening HTML files (which must be one of the supported browsers), and from there it is possible to browse all sub-objects by following the links.

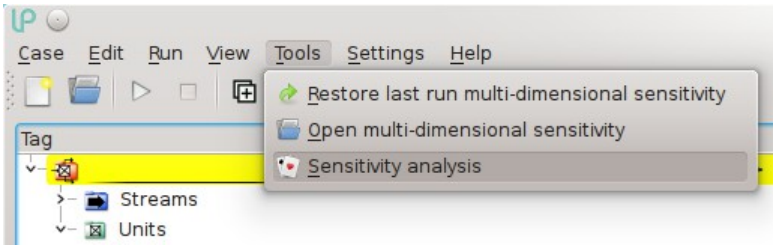
Sensitivity analysis

Very often in the course of a project sensitivity studies need to be performed. These sensitivity studies are very repetitive and only consist in changing one or more parameters (controlled variables) in a certain range for a certain number of points, by running a simulation for every point and recording in a table a certain number of results (monitored variables).

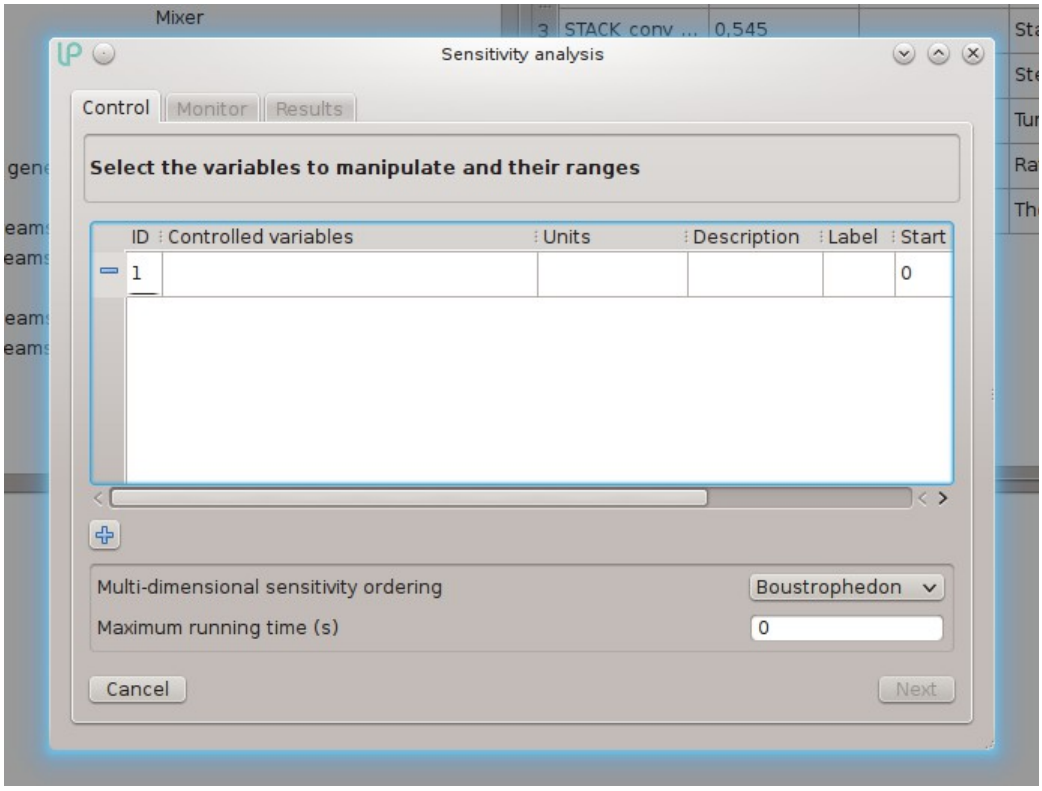
To automatize these tasks the LIBPF™ user interface has a multi-dimensional sensitivity analysis feature. In practice this tool allows you to determine how sensitive a model is to the variation of the values of the parameters and assess how will the variation of the value influence the behavior of the model; it also provides assistance for the selection of the so-called “critical” variables, that is those whose deviation from the nominal value influences the performance indicators the most; with this tool you can acquire a lot of information about the model and the process in a short time.

The sensitivity analysis tool of the LIBPF™ User Interface allows you to carry out several simulations by controlling one or more variables while maintaining all the other unchanged, and monitoring the effect on one or more results.

If you click on Tools → Sensitivity analysis:



a window will appear with three tabs: “Control”, "Monitor" and "Results":



On the "Control" tab it is possible to select one or more controlled variables (at least one is required), setting the units of measurement, the optional label to display in the results table ad column header, the start and end values for the range to scan and the number of points the range must be divided into. The table comes pre-filled with one row, it is possible to add additional controlled variables by clicking on the “+” at the bottom left. It is possible to remove a previously set controlled variable by clicking on the “-” button on the left side of each row.

In the lower part of the window it is possible to set the sensitivity execution order (natural, the default boustrophedon or quasi-spiral) and the maximum running time. The sensitivity execution order is important if there are some regions of the scanned domain where convergence is difficult. The maximum running time, if set to a value strictly greater than zero, is interpreted as a time-out expressed in seconds - if the sensitivity runs for so long, the run is interrupted and the results collected up to that point will be displayed.

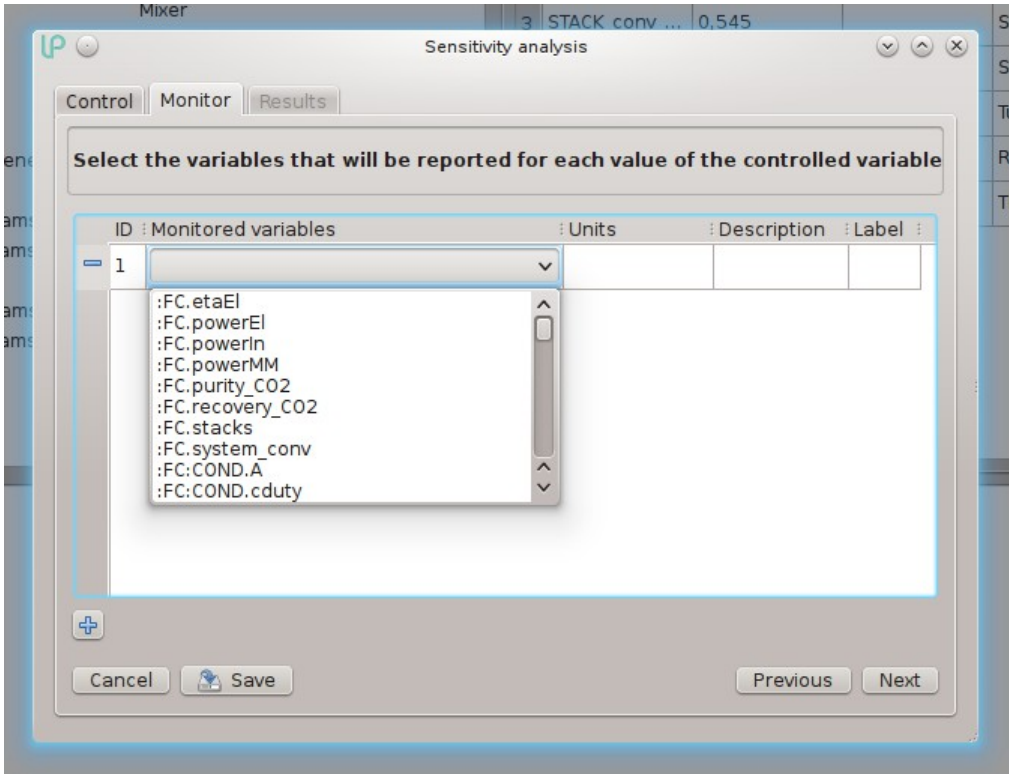
The user can choose the controlled variable from the list of all the variables that can be specified for the current case (these are the variables that appear in the “Input” tab of the units and streams).

As soon as one controlled variable has been chosen, or its selection has been changed, the program updates the units of measurement and initializes the start and end sensitivity limits with the current value of the variable; the description of the variable is also shown. The user must typically only change one of the two limits and probably set the number of points to a value greater than the default value equal to 1 that would reduce the sensitivity to the execution of a single run.

At this point you can press “Next” to proceed to the “Monitor” tab where you can choose the variables (results) to be monitored.

The user can choose the monitored variables from the list of all the results for the current case. As soon as a variable has been chosen, or its selection has been changed, the program updates the units of measurement, the description and the label of the variable. If desired, the user can change the label, which will be shown as a header in the corresponding column of the results table.

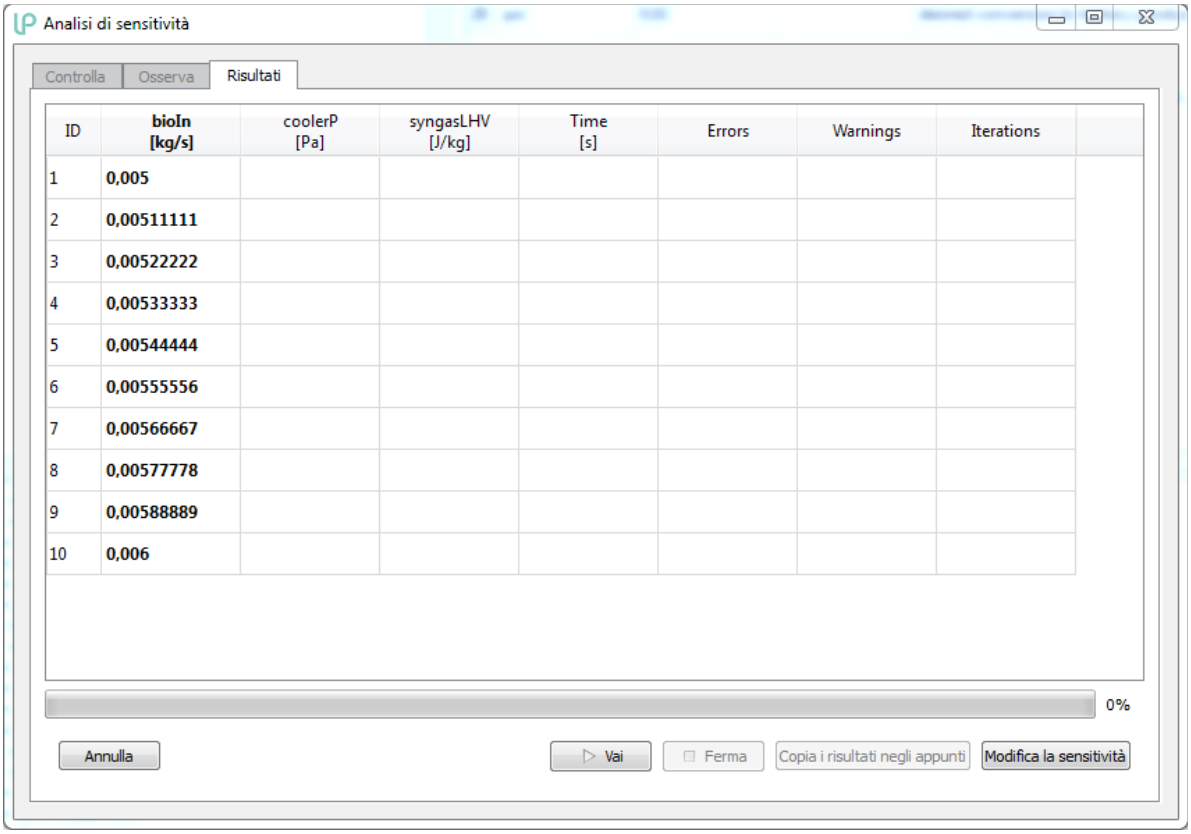
The table of monitored variables has a variable number of rows, however, greater than or equal to one (it does not make sense to follow a sensitivity study without monitoring at least one variable). The user can add new rows or remove the existing ones by using the plus (+) and minus (-) buttons.



At this point you can click “Next” to proceed to the “Results” tab from which you can start the sensitivity analysis by clicking on the “Go” button; before doing so, form this dialog you can also save the configuration of the current sensitivity analysis by clicking on "Save" (see below, "Saving and loading sensitivity analyses").

Note that once arrived at the “Results” tab the two previous tabs are frozen, i.e. the settings for the controlled variable and for the monitored variables can no longer be changed. In fact, the “Edit sensitivity” button functions as a “back” button: unlocks the “Control” and “Monitor” tabs and allows you to change any settings.

If instead a sensitivity analysis is launched, the LIBPF™ user interface starts the calculation kernel. During the execution the rows relative to each value of the controlled variable are highlighted while gradually proceeding to the calculation, and the results of the monitored variables are tabulated as soon as they become available. You can at any moment copy the table (by pressing the “Copy results to clipboard” button), stop (by pressing the “Stop” button) and resume (by pressing the “Go” button) the execution of the calculation.



The rows are color coded highlighted according to the table:

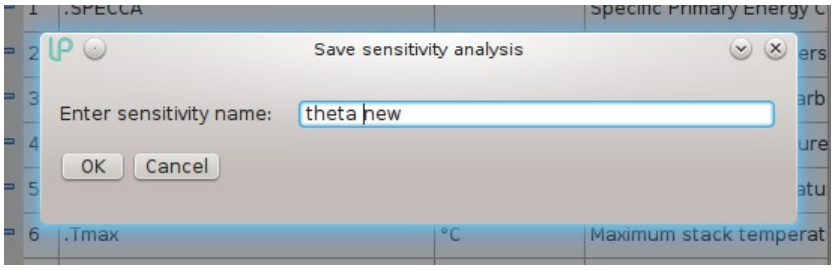
Grey	Row in execution
Green	Row executed without warnings or errors.
Yellow	Row executed with warnings
Red	Row executed with errors (results are available, but probably not valid)
Dark Red	Row not executed because of a serious internal error of LIBPF™ (no results available)
Purple	Row not executed because of a LIBPF™ crash (no result available)
Dark cyan	The row is not completely executed because of an user break (no results available)

The table generated in this way can be copied to the clipboard (by pressing the “Copy results to clipboard”) and from there into a spreadsheet.

Note: at the end of the sensitivity the interface substitutes the value assumed by the controlled variable in the last run in the appropriate Input box so that the loaded case results amended.

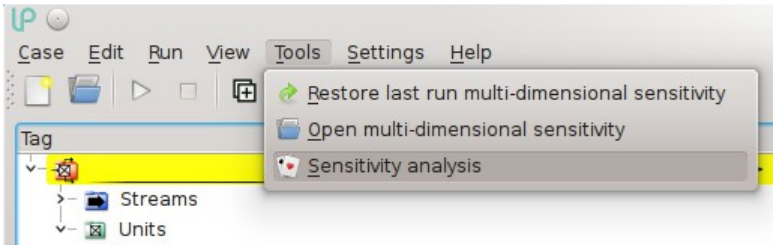
Saving and loading sensitivity analyses

If you click on the "Save" button on the Monitor tab once you have fully specified your sensitivity analysis, a small modal dialog appears:

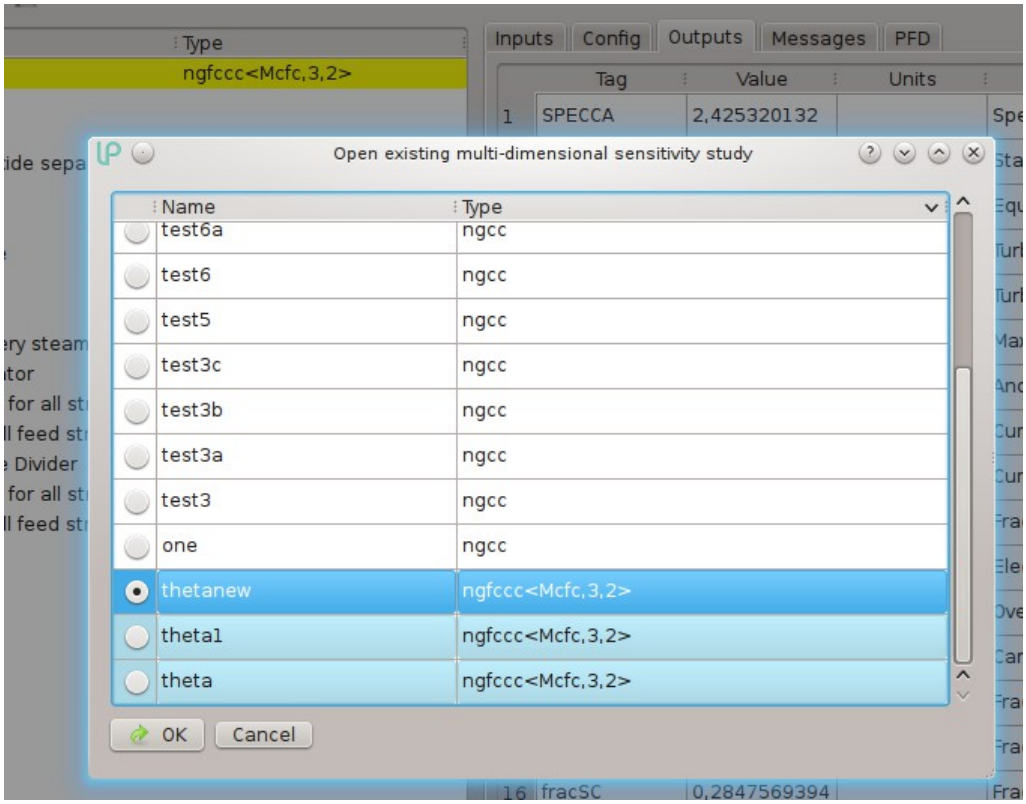


where it is possible to enter a meaningful name for the sensitivity, up to 50 characters long, containing any character except the following reserved characters: < (less than) > (greater than) . (period) : (colon) " (double quote) / (forward slash) \ (backslash) | (vertical bar or pipe) ? (question mark) * (asterisk) _ (underscore), characters whose ASCII integer representations are in the range from 0 through 31 and $ (dollar sign). If the supplied name has already been used to save a sensitivity for the current type, the user is asked for overwrite confirmation, else the sensitivity is saved to an XML file in the working folder, with a full name that contains both the sensitivity name and the current type name.

Saved sensitivity analyses can be loaded back using the "Open multi-dimensional sensitivity" dialog box that is available under the Tools menu:



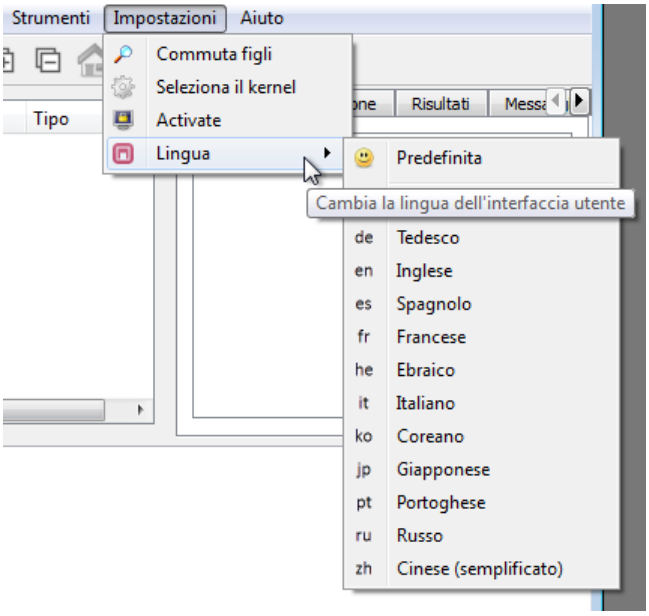
The following dialog box appears:



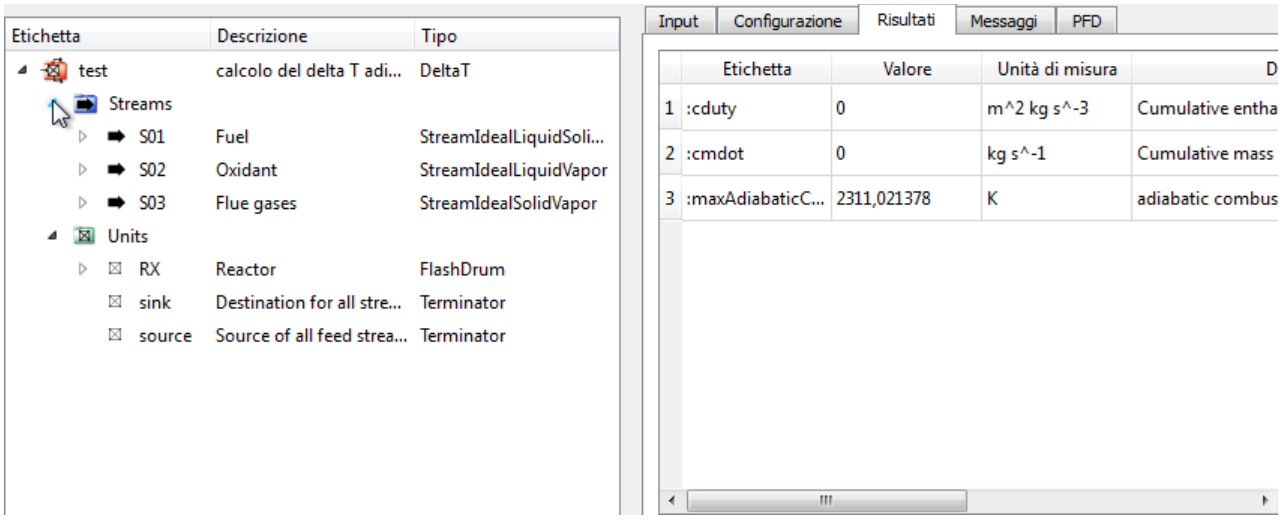
The dialog shows the list of available saved sensitivities along with their model types; the saved sensitivities whose type is equal to the type of the currently loaded case are highlighted in light blue. Typically it makes sense to retrieve a previously saved sensitivity for the same type as the current type, but advanced users can exploit the power of loading an existing sensitivity for a similar type, provided they know how to adapt it if required.

Settings

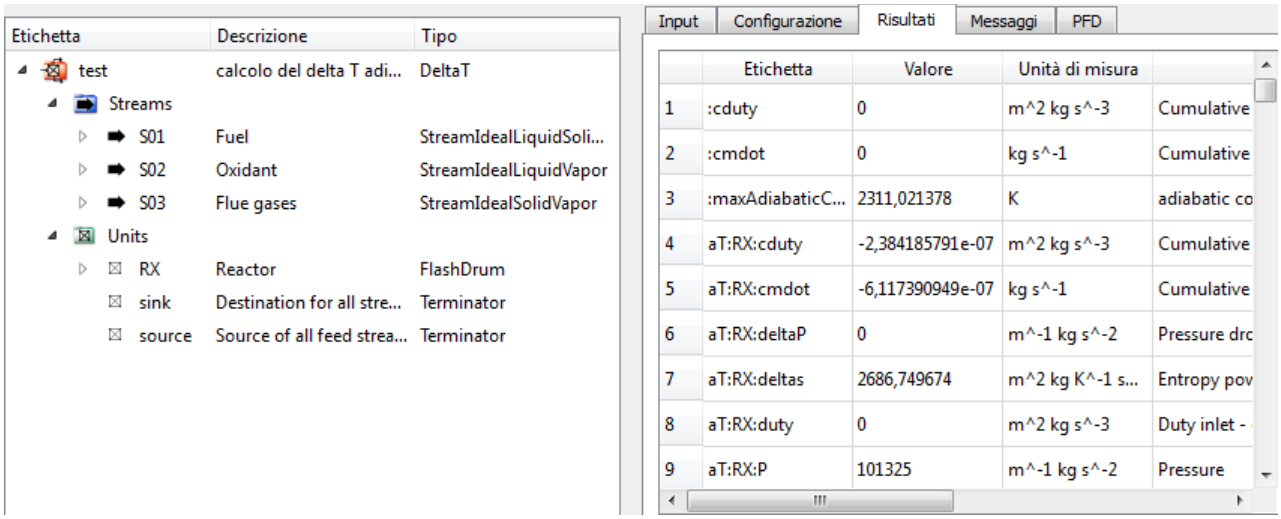
From the settings menu you can change some of the general settings of the application:



- Swap children: toggles the viewing in the details view panel of the input variables and of the results of the objects in the currently selected object in the tree view; for example if the currently selected object is the deltaT flowsheet, and the viewing of the “children” is disabled, the interface could look like this:



if instead the viewing of “children” is activated, the interface could look like this:



note how in the details view panel the results of the internal objects of the flowsheet have appeared, recognizable because the label contains the complete path to them (e.g. RX:P is the pressure of the RX unit);

- Select the kernel: if more calculation kernels have been installed (each of which can simulate various components and processes) this command allows you to switch from one kernel to another; note: this feature is only available on Windows systems;
- Activate: allows you to start the automatic activation procedure (see the LIBPF_USR_activation);
- Language selection: from here you can change the language of the user interface (the default is set to the language of the operating system); note: the language selection is only effective after restarting the LIBPF™ user interface.