T H E R M O P T I M ®

ADVANCED
MODELING
HINTS

JAVA VERSIONS

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CONTENTS

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Model construction and verification methodology

Thanks to their powerful modeling environments, simulators as Thermoptim allow quick development of possibly very complex energy systems models. They can lead to significant productivity gains, but on one condition, that is to be used wisely, which means to avoid a number of pitfalls that their apparent ease of use can mask .

To truly take advantage of their potential, we must take a number of precautions, or, if you prefer, you need a good methodology for the construction and verification of models. The purpose of this note is to provide Thermoptim users with a number of recommendations based on past experience.

Think before you start entering the model

One of the most common errors made by first-time users is to start making their model before thinking through what they want to do. They open the software and start building a diagram without really knowing where they are going with it.

It is extremely important to start by having a good understanding of the problem at hand: What is the problem, what results are we looking for, what information do we already have, what information are we missing, what thermodynamic components must we use, what global architecture, what fluids are we working with, are there any state changes or chemical reactions (combustion, etc.), will the components of Thermoptim basic set be able to represent the fluid changes? At this point it is often necessary to reformulate or even transform the initial problem statement, and a sheet of paper or a whiteboard can come in handy.

Once the problem is defined, we can try to make it less complex by breaking it down into simpler parts, then rough out a solution using simplistic hypotheses to analyze each of the parts (perfect gas), and perform dimensional analyses, in order to get an idea of the orders of magnitudes of the flow rates and energy involved.

Build the model in several steps, and perform calculations step by step

Only after this preliminary work can you begin to build the model in Thermoptim, if possible proceeding by iterations: resolve the sub-problems identified beforehand and check the consistency of the results for each one (especially the mass and energy balances), if necessary build external components, then assemble the full model and check for validity.

When building the model, we recommend saving the different versions of the project and diagram in separate files, to safeguard against data loss due to an input error, software error or computer error, and also so you can go back to a previous version if necessary.

It is also important to document the model as thoroughly as possible, both globally and in detail. In the different primitive types of Thermoptim, except the substances, there is a comment field where you can provide information on the meaning of a parameter setting, or the role of a point or a process. In the diagram editor, you can easily add text to distinguish the main groups of components representing the parts of the model. The documentation work is always easier to do when the model has just been built, rather than several months later. It's also much easier to work with a documented model that provides information on the choices made than to try to remember why you did what you did at some later date.

Until your model has been checked (next step), it is better not to use the automatic recalculation engine, but rather to perform the calculations one by one, component after component, following the flow logic of the fluids used. In this way, you will not automatically spread errors that may skew all of your parameter settings.

Restart Thermoptim after building a somewhat complex model

Despite all precautions taken in developing the software, experience has shown that the simulator can behave oddly, especially when performing automatic recalculations, when you build a model for the first time. These problems disappear when you restart the program.

So get in the habit of saving your work, i.e. the project and diagram files, and then exit Thermoptim, whenever you create a new model, especially if you start from an existing model and add or delete components or if you rename a file. Re-open and reload your model. This will eliminate any problems that arise when working with a new model.

Test the model very carefully before using it

If the model contains a large number of components, there are numerous possibilities for error:
- errors in representation of the global architecture
- errors in connection of the points to the processes
- errors in the logical or thermodynamic parameter settings of the components

Consequently it is necessary to thoroughly test the model by checking that its structure is correct and the results are consistent, specifically with the orders of magnitude identified during your initial reflections. Thermoptim already performs various checks during the input phase, and displays messages when it detects a problem, but there are many errors that only the model designer can identify.

To facilitate this difficult step, the software provides the user with various functions (Diagram/Simulator interface, substance manager, interactive charts) and also has diagnostic tools in the standard version, accessible from the Special menu from the main project window.

Useful to know tips

We give here a series of tips (which are explained in the reference manual) whose knowledge can help save lots of time when using Thermoptim to model energy systems a bit more complex than the basic examples.

## Limitations of the automatic propagation of point names and substances

Most components of the Thermoptim core only involve one substance, and accept as an entry point the exit point of the component just located upstream. This is why, to simplify the entry of a component in the diagram editor, you may in the general case define this component by typing firstly its name, and secondly that of the exit point. When you connect to it the upstream component, the name and the substance of the inlet point are automatically updated.

This rule, however, is not observed in a few cases:
- In the components which involve a substance different in the output and the input, such as a combustion chamber, or an external process

- In the downstream components of a mixer, since on the one hand there may be change in substance composition, and secondly there are several points upstream
- In the two points downstream of a separator, wherein the substance is the same, but with two different states of the inlet point

Entering the name of the substance is made in the component property definition screen.

Entering the name of the substance for combustion
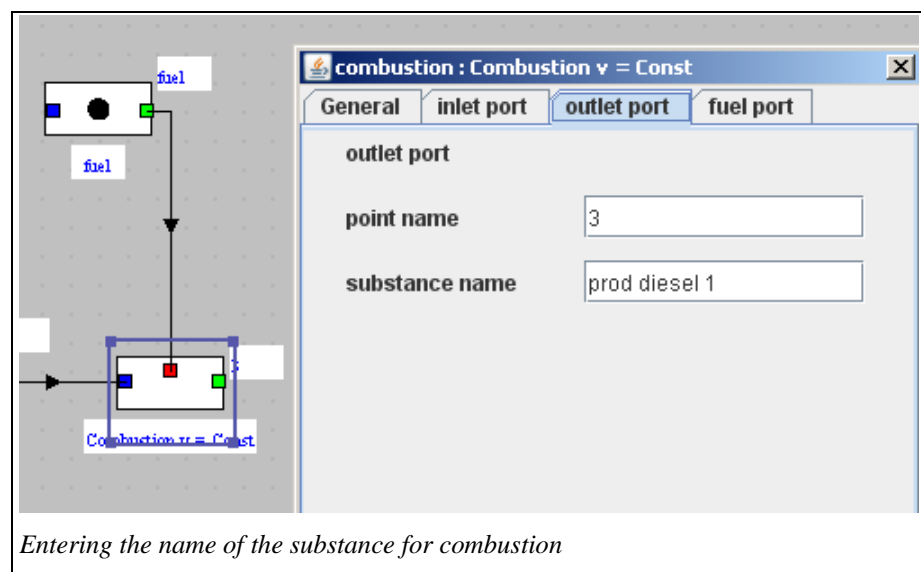
For combustion processes, it must be done in the tab of the outlet port, if possible before connecting the combustion chamber downstream, so that the substance can be subsequently propagated downstream.

In the case of a mixer, the input must be made in the tab of the main vein component inlet port, located downstream.

Entry of point and substance names at the mixer outlet

Connections between two nodes
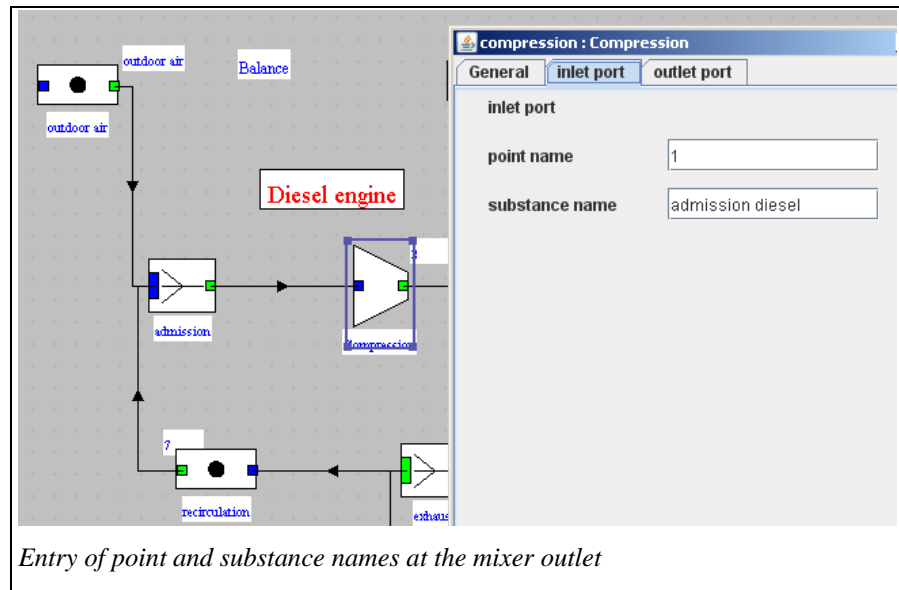
Since it is impossible to connect two nodes together, a process - point is automatically created between them when attempting to do so. Then just set it to complete its definition.

Setting combustion, compression or expansion processes

The explanations for setting the combustion, compression or expansion processes are given respectively in Diapason sessions S15En for the first and S11En for the others, and in Volume 2 of the Reference Manual .

These resources can be accessed directly from the links below[1].

Setting heat exchangers

The explanations for setting heat exchangers are given for exchange processes in Diapason session S10En, and for heat exchangers in session S18En and in Volume 2 of the Reference Manual.

These resources can be accessed directly from the links below

Renaming elements of an existing project

It can be very economical to start from an existing model and modify it, but certain precautions must be taken to avoid spending hours testing the new model. In particular, it is necessary to be very careful when renaming substances, points and components. We strongly recommend using the "Rename" function (Ctrl R) accessible from the substance manager (see below) for substances, and the diagram editor for the others, because it changes the name not only in the primitive type selected, but also in all those that are logically connected to it.

To rename a process, select the component in the editor, and press Ctrl R or select the line Rename from the Edit menu. A window showing the existing name is prompted, inviting you to enter a new name, which of course must not to have already been assigned to another process.

To rename a point, select the link between two components corresponding to this point, and operate similarly.

You have probably noticed that the name field of a point between two processes is not editable in the properties screen of a component port, in order that you cannot enter two incompatible values between the outlet and inlet ports of the two connected components. The only way to make this field editable again is to disconnect the process.

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[1] http://www.thermoptim.org/sections/logiciels/divers-portail/seances-disponibles

Substance manager

The Substance Manager, accessible from the
Special menu of the simulator (except in the
demo version) displays all of the substances
used by the project. If you click on one of
the lines, the points linked to this substance
are displayed in the table below. This makes
it easy to check the substances used in the
projects and the points linked to them.

If a substance is not linked to any point, it
can be deleted. If a line is selected and you
click on "Display substance properties", its
composition is displayed if it is a gas, and its
typical parameters are displayed if it is a
vapor.

You can also replace a substance throughout
the project, for example to test the effect of a
substance change. For example, by
considering the influence of Cp variation
with temperature for ideal gases, you may obtain analytical results.

Substance manager
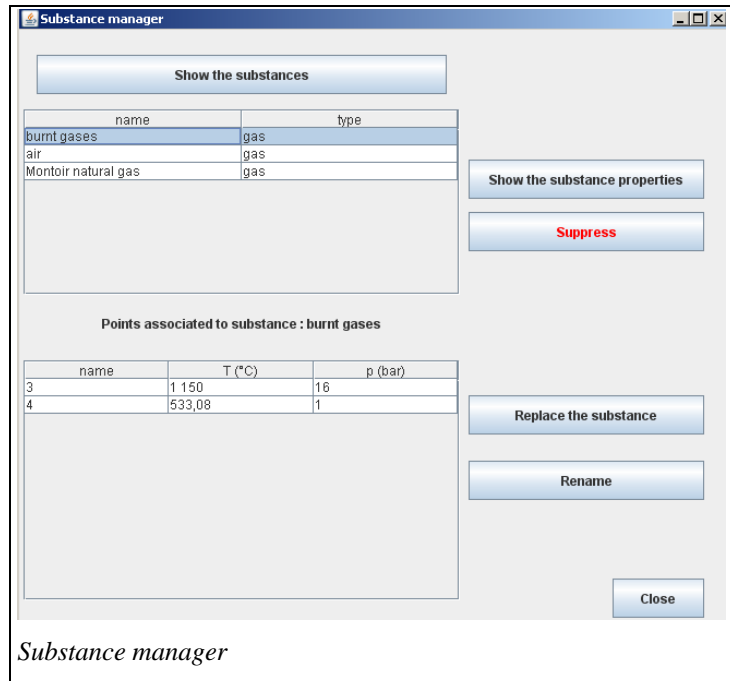
You can only rename a substance if it is not a vapor. Obviously, the new name must not be the name of a pure or
protected gas or a vapor.

Some substances exist as pure gases and vapors, under two different names, one being the common name, the
other the chemical formula. It is indeed the same substance, but represented by different models. For example,
the steam "water" provides information on the properties of water around its liquid - vapor equilibrium curve,
while the pure gas "H2O" is modeled as an ideal gas (and therefore never condenses).

Gas "H2O" can enter into the composition of any compound gas, such as a product of combustion, while steam
"water" cannot be mixed with other substances.

The zero reference for the ideal gas enthalpy is 1 bar and 25 °C, while for each steam it is specific.

Troubleshooting models

To help diagnose the differences between the diagram editor and the simulator, their interface has been
supplemented by two red buttons, allowing on the one hand to find modeling anomalies, and secondly to delete
those selected (last column checked).

Modeling anomalies include:
- The elements of the simulator absent from the diagram editor
- The elements of the diagram editor absent from the simulator
- unconnected points present in the simulator
- substances unused

The implementation of these new features is quite simple: by clicking on the button "Search anomalies " all
questionable items are displayed in the list. Clicking on the "Delete anomalies" button offers to delete the
selected items only.

Note that once some elements deleted, new anomalies may appear, as new unconnected points or unused
substances which used were before deleting points . It may be necessary to iterate for all deficiencies to be
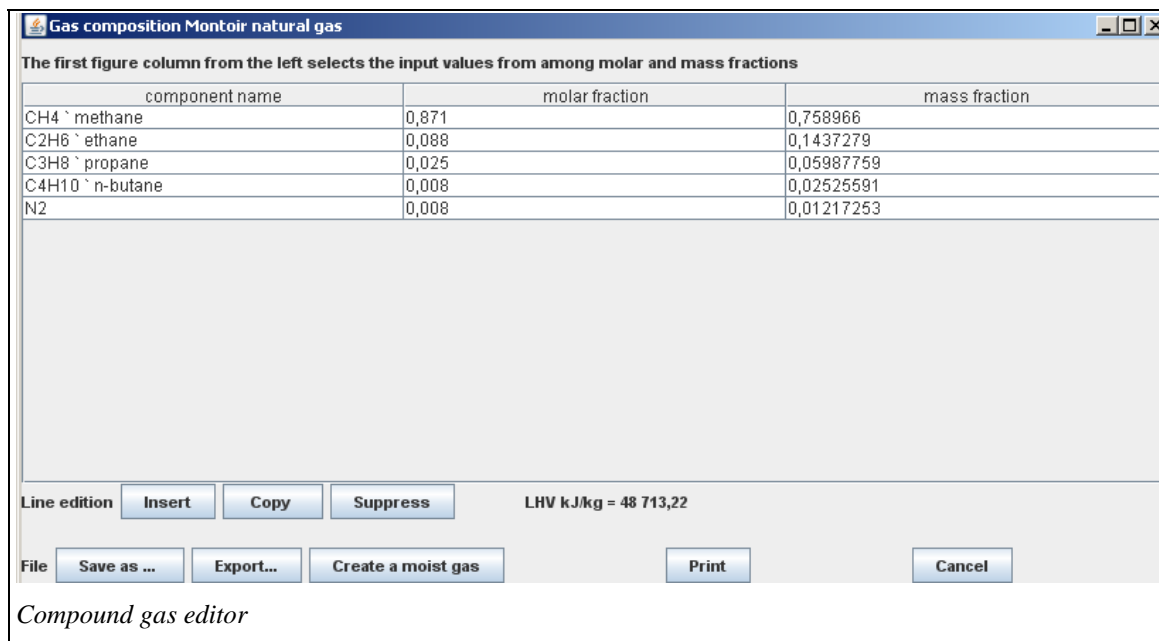removed.

To avoid any unwanted operation buttons to update the simulator and diagram editor are disabled when you click
on the search of abnormalities, and that to remove anomalies when using the interface in the usual way.

Diagram Interface / Simulator version 1.5
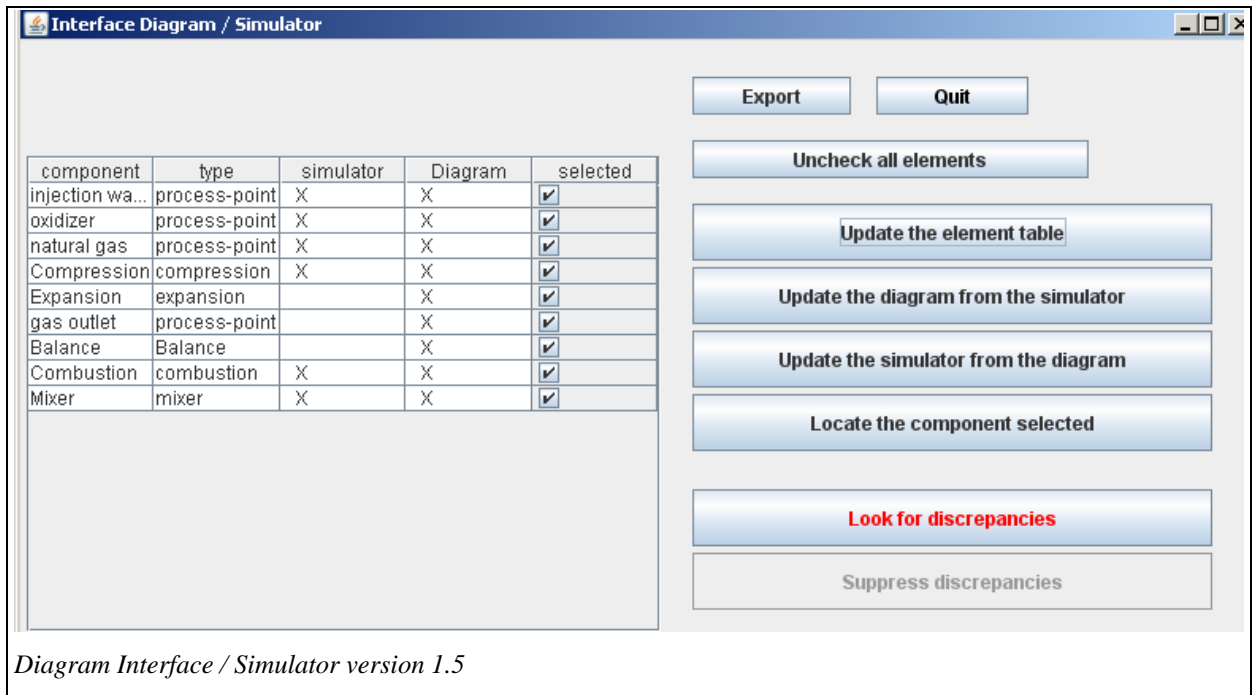
Compound gas editor

To define a new gas compound in Thermoptim, just give it, in the diagram editor, a name that is not that of a pure gas or vapor. When transferring into the simulator, a default composition is then provided, waiting to be recalculated later. It is also possible to enter a name in the substance field of the point screen and then tap Enter. The new substance is instantiated by default.

In Thermoptim the gas composition is obtained by clicking on the "view" button next to the name of the substance in the point screen.

The first figure column from the left selects the input values from among molar and mass fractions

component name	molar fraction	mass fraction
CH4 ` methane	0,871	0,758966
C2H6 ` ethane	0,088	0,1437279
C3H8 ` propane	0,025	0,05987759
C4H10 ` n-butane	0,008	0,02525591
N2	0,008	0,01217253

Line edition   Insert   Copy   Suppress   LHV kJ/kg = 48 713,22

File   Save as ...   Export...   Create a moist gas   Print   Cancel

Compound gas editor

It appears in the gas compound editor that provides several features to save, delete, export or import gas compounds in the package database.

It is possible to change the composition of the gas, choosing names of components from the list of pure gases proposed in the left column, and entering either the mole fractions or mass fractions. Once set, the gas can be:

- saved by clicking "Save". The software verifies that the sum of the fractions of the column of numbers on the left is equal to 1, and saves the gas. If the sum differs from 1, nothing is done. Only unprotected gas can be saved.

- renamed by clicking "Save As...". The test on the sum of the fractions is made, and the gas saved under a new name that you are asked to give.

- Exported by clicking on "Export...". The gas composition is then copied into a text file with the name you give, and you can open it with a word processor or a spreadsheet. For example, the previous gas can be exported in the following format:
- It is also possible to create, from the gas displayed in the editor, a moist gas of given absolute humidity. To do this, click on "Create a moist gas". The software prompts you for the name of

	A	B	C	D	E
1	THERMOPTIM INTERACTIVE CHART. Copyright 1998-2005 R. GICQUEL				
2	Compound gas file	2 septembre 2013 17 h 02 CEST			
3					
4	Gas name	Montoir natural gas			
5	Number of components	5			
6	component name	molar fractic	mass fraction		
7	CH4 ` methane	0.871	0.758966		
8	C2H6 ` ethane	0.088	0.1437279		
9	C3H8 ` propane	0.025	0.05987759		
10	C4H10 ` n-butane	0.008	0.02525591		
11	N2	0.008	0.01217253		

Gas composition file

the gas and the absolute humidity that you want, then builds a new compound gas, with the same dry gas as well as the one from the editor, and absolute humidity equal to what you entered. This gas is added to the list of gas compounds of the database.

- Finally, if you cancel, the compound gas editor is closed.

Pressure control: isobaric exchange processes

In Thermoptim pressure choice is normally left to the discretion of the user, knowing that all points are initialized by default at 1 bar and 300 K. It is possible if desired to make isobaric the "exchange" processes. This requires first to check "Isobaric exchange processes" in the global settings screen, as it is not check by default. When selected, the "exchange" process screen shows an iso-pressure option checked by default when creating a process, and saved according to the user's choice. When this option is visible and checked, the pressure of the upstream point is automatically propagated to the downstream point. Otherwise nothing is done.
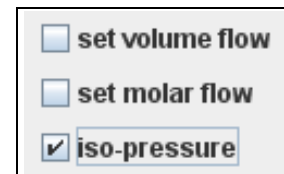
By operating this way during the creation of a new diagram and a new project, the pressure of the downstream point of an exchange process is automatically updated at the same value as that of the upstream point when the process is calculated.

Flow control

Flow rate control is extremely important in practice. In Thermoptim, it is done by the nodes and the process connections.

In mixers and separators, the flow rate propagation is rather simple: in a mixer the main vein flow rate is the sum of all branch flow rates, and in a separator it depends on the quality of the two phase fluid entering the node and on the node effectiveness. In a divider, the distribution of the main vein flow rate in the different branches is made proportionally to their flow factors.

In a divider the distribution of the flow rate of the main vein between the branches is generally made proportionally to their flow-rate factors. There is however an exception: it is possible to set the flow rate in a process at the outlet of a divider, provided that this node has two branches, that with the set flow rate, and

another one. In this case the flow rate of the second process is set equal to the flow rate of the main vein, minus that of the branch with the set flow rate, and the flow-rate factors are recalculated accordingly. In this case (as in the previous example) the message "set flow" is displayed in red below the name of the main vein.

Flow rate can also be automatically propagated between two processes when the following rules are met:

- first, it is necessary to ensure that the two processes are connected together and with no other type. If a point is connected to but one process as an inlet point and to but one process as an outlet point, it is considered as straightly connected. This information can be retrieved from logical connections between the types.
- second, the automatic flow rate propagation scheme has to be enabled by checking the "autoflow" checkbox which is located close to the "Recalculate" button of the main project frame
- third, one may wish at the same time to enable the automatic flow rate propagation in most processes and to disable it in some of them. This is particularly useful when there are loops in the process networks. It can be done by checking or unchecking the "set flow" checkbox which appears in each process frame close to the "Delta H" field. When the "set flow" checkbox of a process is on, its flow rate remains unchanged, except if it is connected to a node.
- it is also possible to retrieve information on connections between processes from the diagram editor as explained below in the section entitled "Flow rate propagation in complex cycles".

To summarize, when two processes are straightly connected, the flow rate of the upstream process is automatically propagated to the downstream one, provided the autoflow is on and the latter's flow rate is not set.

Volumetric and molar flow rates

It is also possible to display or hide the volume and molar flows. To display them, select the "Show volume and molar flows" in the global settings screen (Help menu).

By displaying them, you can enter the values of set rates in volume and molar values in all exchange processes or process-points, which can be interesting in a number of cases. To allow the entry of volume and molar flows, the "exchange" process (and process-point) screen has been changed.
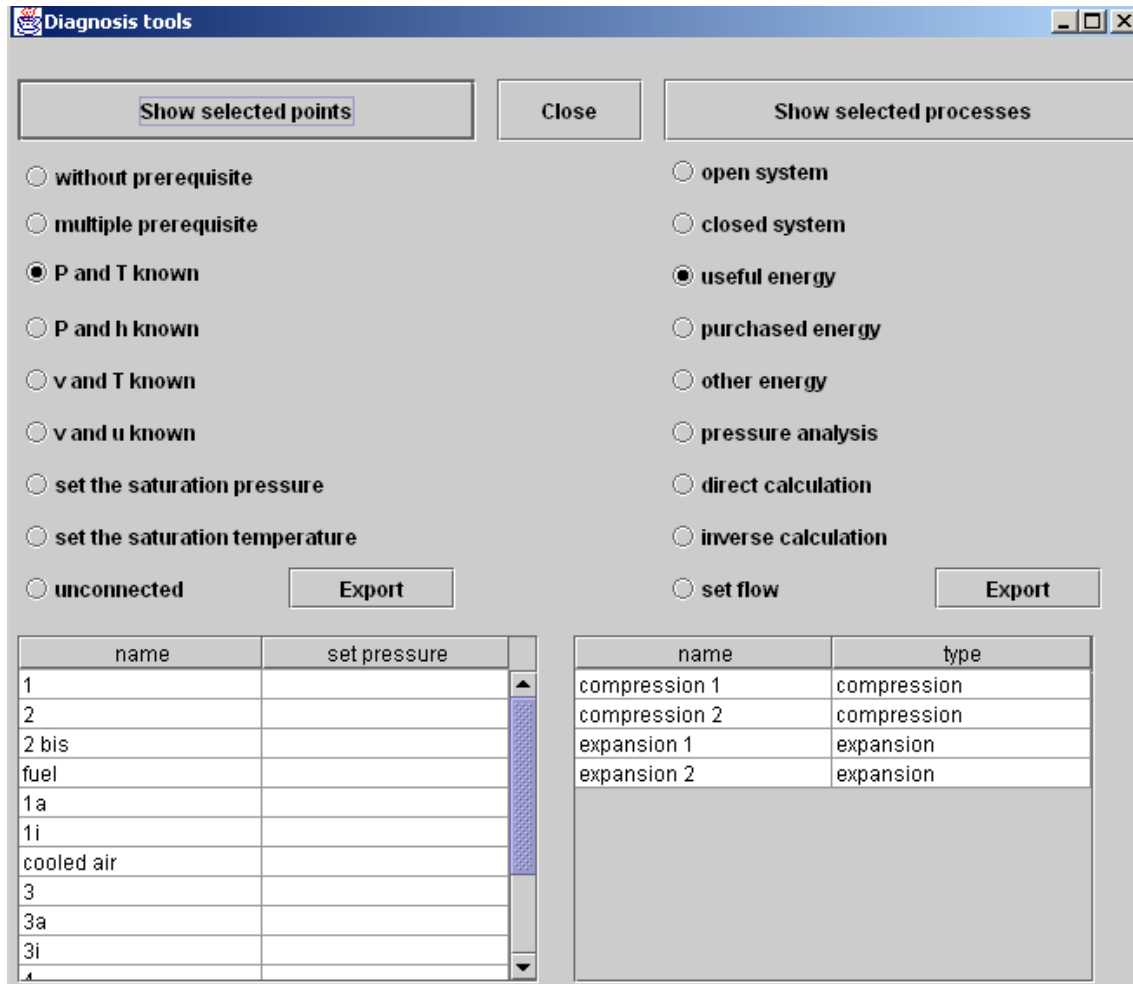

Exchange process screen a with volume and molar flow rates and flow units

Two fields and two options allow you to enter either the volume flow rate or the molar flow rate (by default the mass flow rate is taken into account). In all cases, the two rates which are not specified are based on the third.

To avoid conflict with the mechanism managing the automatic propagation of the flow, it is possible to set the volume or molar flow only in the processes with set flow rate. If you select one of these two options and the flow rate of the process is not yet set, a message notifies you of the problem and asks you to verify that the set flow option is consistent with your model. The flow is then set without the possibility for you to change this option unless you deselect the volume or molar set flow rate options.

Diagnostics

For those who have a standard or higher version, it is recommended to start testing using diagnostic tools (Special menu simulator) to check that the setting of a point or one of the processes has not inadvertently been wrong (just because of an error click). Consider in particular the calculation method (direct, inverse, open or closed system ...), the types of energy that affect the balance sheet...

Diagnosis tools		_ □ X

Show selected points	Close	Show selected processes

Points		Processes	
○ without prerequisite		○ open system	
○ multiple prerequisite		○ closed system	
● P and T known		● useful energy	
○ P and h known		○ purchased energy	
○ v and T known		○ other energy	
○ v and u known		○ pressure analysis	
○ set the saturation pressure		○ direct calculation	
○ set the saturation temperature		○ inverse calculation	
○ unconnected / Export		○ set flow / Export	

name	set pressure		name	type
1			compression 1	compression
2			compression 2	compression
2 bis			expansion 1	expansion
fuel			expansion 2	expansion
1a				
1i				
cooled air				
3				
3a				
3i				

For points, the search options are as follows:
- **no prerequisites** other than the substance that is linked to them or a set pressure: theoretically, these points are never modified, unless the composition of the linked substance changes or if the set pressure is changed.
- **multiple prerequisites:** if a point has more than one prerequisite, it means that it can be modified by more than one component. This is generally because, during modeling, it was incorrectly connected either to the outlet of two different transformers, or to the outlet of one transformer and the inlet of the main transformer of a mixer.
- calculated in **open system with either p and T or p and h known**.
- calculated in **closed system with either v and T or v and u known**;
- with a **set saturation pressure** or **a set saturation temperature**;
- **not connected** to a process: these points are not used and can generally be deleted.

For processes, the search options are as follows:
- **open or closed system;**
- **type of energy: useful, purchased or other**;
- **pressure analysis:** in Thermoptim, the pressures are initialized by default at 1 bar, then the user must set the values, since the software does it in only a very few instances. If the user forgets to do so or makes an error, convergence problems may appear. This search option covers on the one hand all of the processes other than compression, expansion and throttling in which the outlet pressure is either greater than the input pressure

(physical impossibility except for certain external processes), or less than 80% of the inlet pressure (excessive pressure drop), and on the other hand all of the nodes through which the pressure increases (physical impossibility except for certain external nodes).

- **direct or reverse calculation;**
- **set flow rate:** this option facilitates checking of flow rate propagation consistency in complex projects.

You can double-click on the two tables. If you double click on one of the lines, the corresponding components are displayed. By clicking on "Export", you print the list of points or processes to the file "output.txt".

In the screenshot above, there is 1 point with multiple prerequisites, and the right part of the screen shows the result of a pressure analysis.

Point with multiple prerequisites

Double click on the line of the point "COLD RH" to display its screen and access the links window (see the paragraph "Links Browser" in the next section).

By looking at the prerequisite elements, we see that that "COLD RH" is defined both as an outlet point of the "HP TURBINE" turbine and as an inlet point of the main process of the mixer "FROM HP TURBINE & GAS…", which is a modeling error that would have been difficult to detect without the diagnostic tool.

Links browser

Pressure analysis:

The pressure analysis has identified six components that may have incorrect parameter settings. Double click on the table on the right to display their screens. For the first three, the outlet pressure was rounded up, and the error is negligible.

The next two components are external processes corresponding to a non-adiabatic compressor and a non-adiabatic turbine, so it is perfectly normal for the first component's downstream pressure to be greater than its upstream pressure, and for the second component's downstream pressure to be less than 80% of its upstream pressure.

As for mixer "MIX2", the pressure upstream of its main process is greater than the downstream pressure of its branches, which is clearly an error in parameter setting.

Thus, the diagnostic tool identified three negligible errors, two normal pressure changes in external processes, and one parameter setting error at the outlet of a mixer. Since the project involves sixty or so points and processes as well as fifteen or so nodes, identifying these errors would have been difficult without this tool.

Testing the automatic recalculation

If everything looks good after these checks, save your model, then test it in automatic recalculation mode. This step, as we have said, should not be done too early, with a model that has not undergone previous tests. In contrast, a model without error recalculates without difficulty, and the recalculation engine can perform various sensitivity analyzes which are very useful to assess its validity.

If you want the flow rates to be automatically propagated, check that the "auto flow" option is selected, that the set flow processes are specified, and test the consistency of your model using the diagnostic tools.

Once you have verified the model, open the recalculation tools screen, and click the "Recalculate" button if the number of computable types is not zero. Otherwise, you must first calculate an upstream element.

When you use the automatic recalculation mechanism, invalidated computable types are calculated in turn, possibly in parallel. Once an item is calculated, subordinates are invalidated, making the process iterative. When all the items which were initially computable are recalculated, the overall balance is performed and the values of the indicators are updated. Generally, new items were invalidated. Iterate until the indicator values stabilize (5-10 iterations suffice most of the time).

If the process does not converge, it is likely that there is a problem with interconnections or flow propagation: it may be necessary to set the flow of one of the processes, especially in the different loops.

From the Professional version, the screen of the optimization method allows you to automate repeated recalculations with stopping criteria related to the convergence of the model.

If you select the "locked" option, the invalidation mechanism is blocked, which means that when an item is recalculated, it remains valid, even if one of its prerequisites is disabled. This completes the process of recalculation few iterations.

If difficulties arise during automatic recalculation, it usually means either that the thermodynamic setting is not good, or the model itself needs to be reviewed.

Although the mechanism of automatic recalculation gives good satisfaction, it sometimes happens that some components (such as heat exchangers) are forgotten in recalculations, unless special precautions. This is particularly why a new feature has been added: the multiple selection recalculation scheme explained below.

Recalculating multiple selections

A special method is used to facilitate work on multiple component selections. It is accessible from the Special menu of the diagram editor.

When a multiple selection is done, it can be loaded in this screen by clicking on the button "Update the selection from the editor".

The list of elements selected (points, processes, nodes, heat exchangers) appears in a table. The order of these components can be changed using the

Multiple selection management screen

scroll buttons located in the lower right part of the screen, and elements can be deleted.
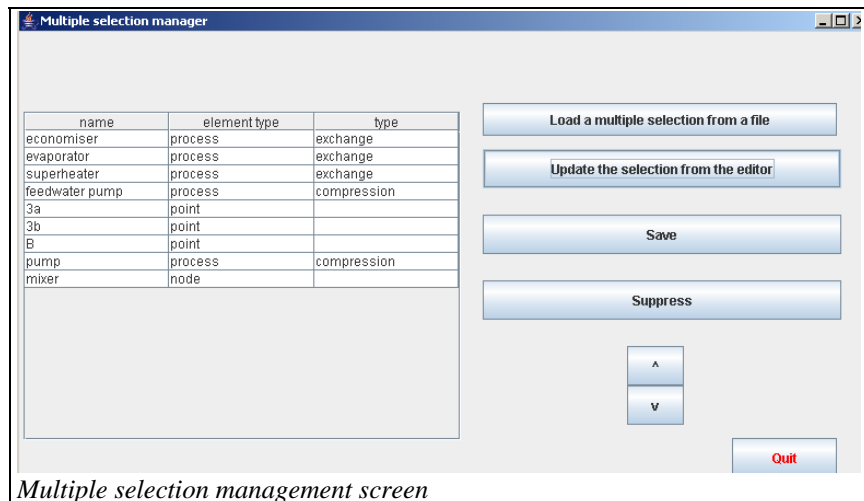
The list of elements selected (note: for the time being, the points are not selected when the file is re-read) can be saved in a file in the "res" directory. This list can be reloaded by clicking on the button "Load a multiple selection from a file".

Once the selection has been made, various functions can be activated from the diagram editor:

- F5 launches an automatic recalculation in the simulator;
- F6 updates the multiple selection management screen by loading the current selection;
- F7 recalculates the different elements in the selection, in the order in which they appear on the multiple selection management screen. The values of the points selected will be updated if the values are displayed.

Sélection multiple

- F8 selectively displays or hides the values of the points on the multiple selection management screen. To display the values, type F6, then F3 twice (the first time selects all, and the second the multiple selection). Then, each time you recalculate using F7, the values displayed are updated.
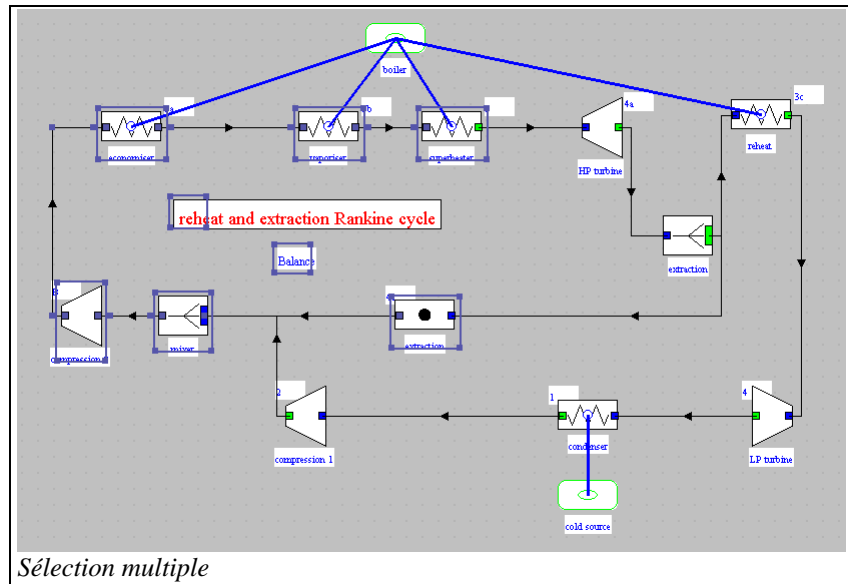
Thus, by clicking once on the F7 key, then press the F5 key, the recalculation of the selected items is performed and then the whole project .

Calculation of exergy balances

A line of the "Result Files " menu allows you to conduct exergy calculations ("Export exergy calculations"). When this menu item is selected, a screen prompts the value of the environment temperature which is defined in the global settings. This value can then be changed, and all the project points and processes are recalculated and stored in a file. Once the calculations done, the environment temperature is set to its original value.

It is thus possible to calculate all exergies brought into play in a project without having to recalculate it completely.
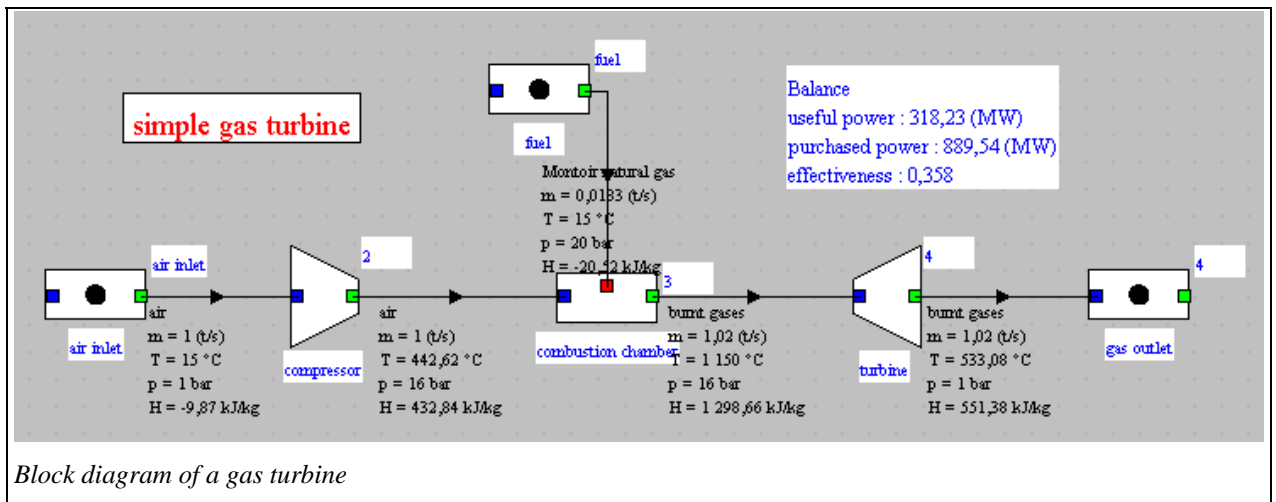
Display Options

Introduction of flow and power units

In order to display the flow and power units, it is possible to choose the unit of flow, from a drop-down list at the bottom right of the screen simulator.

Once this choice is made, the power unit can be displayed on the balance sheet component of the diagram editor, and in the screens of processes.

Choice of flow unit

Block diagram of a gas turbine
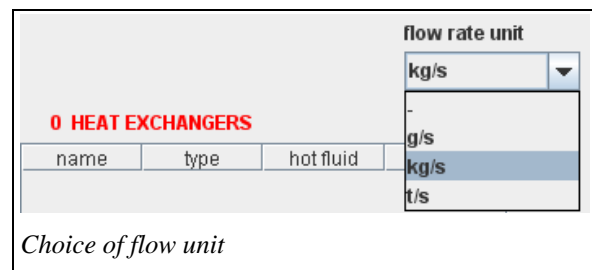
The selected flow unit is saved in the project file.

Change of display options for recalculation

It is possible (if the files are present) to get online access to the documentation in two languages: French and English. The choice is made in the Global settings screen, or by choosing Fr or En as documentation language.

Global settings screen

To simplify the display, it is possible to choose to display or hide certain fields, such as **calculable or invalidated** types.

By default, these fields are not displayed in the simulator. To display them, select the "Display recalculation informations" in the global settings screen (Help menu).

Note that by default, automatic recalculation is enabled, as well as the flow propagation.
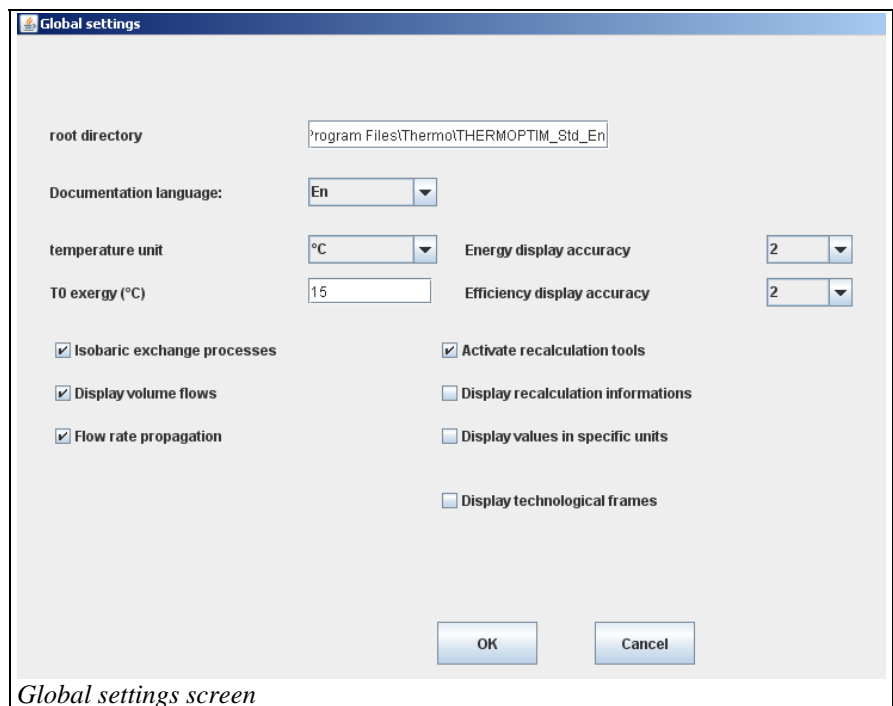
In the balance sheet, it is possible to set the display the precision of energy values in play and effectiveness .

In fields that can be used to enter input values, however, it is however necessary to keep a large number of decimal digits, otherwise the results of the calculations would progressively derive if the calculation options were changed.

By default, the display is 0 decimal digits for energy or power, and 2 for efficiency.

Access the documentation via hypertext links

Hypertext links provide direct access to the documentation and the FAQ. In order for the links to work, the file paths must be identical to what was entered in Thermoptim, otherwise they will not appear on the list.

The documentation in English must therefore be structured as shown in the figure above. If you have an older installer, rename the files accordingly.

Reference manuals

The documentation is located in subdirectories doc_En and doc_Fr of the installation directory

Documentation language: En

Reference manual part 1

Reference manual part 2

Reference manual part 3

Vapor charts reference manual

Ideal gas charts reference manual

Psychrometric charts reference manual

Hyperlinks to the documentation

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